=> file registry
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STRUCTURE FILE UPDATES: 15 NOV 2007 HIGHEST RN 953991-83-8 DICTIONARY FILE UPDATES: 15 NOV 2007 HIGHEST RN 953991-83-8

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http://www.cas.org/support/stngen/stndoc/properties.html

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FILE COVERS 1907 - 16 Nov 2007 VOL 147 ISS 22 FILE LAST UPDATED: 15 Nov 2007 (20071115/ED)

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This file contains CAS Registry Numbers for easy and accurate substance identification.

'OBI' IS DEFAULT SEARCH FIELD FOR 'ZCAPLUS' FILE

=> d stat que L28

L26 104 SEA FILE=ZCAPLUS ABB=ON PLU=ON MASAOKA S?/AU L27 6 SEA FILE=ZCAPLUS ABB=ON PLU=ON IWAZAKI H?/AU L28 1 SEA FILE=ZCAPLUS ABB=ON PLU=ON L26 AND L27

L26 104 SEA FILE=ZCAPLUS ABB=ON PLU=ON MASAOKA S?/AU
L31 242547 SEA FILE=ZCAPLUS ABB=ON PLU=ON BORON/BI
L32 2 SEA FILE=ZCAPLUS ABB=ON PLU=ON L31 AND L26

=> s L26,L31 and L25

L46 2 (L26 OR L31) AND L25

=> file wpix

FILE 'WPIX' ENTERED AT 12:15:52 ON 16 NOV 2007 COPYRIGHT (C) 2007 THE THOMSON CORPORATION

FILE LAST UPDATED: 13 NOV 2007 <20071113/UP>
MOST RECENT THOMSON SCIENTIFIC UPDATE: 200773 <200773/DW>
DERWENT WORLD PATENTS INDEX SUBSCRIBER FILE, COVERS 1963 TO DATE

>>> IPC Reform backfile reclassification has been loaded to September 6th 2007. No update date (UP) has been created for the reclassified documents, but they can be identified by 20060101/UPIC and 20061231/UPIC, 20070601/UPIC and 20071001/UPIC. <<<

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http://www.stn-international.de/training center/patents/stn guide.pdf

FOR DETAILS OF THE PATENTS COVERED IN CURRENT UPDATES, SEE http://scientific.thomson.com/support/patents/coverage/latestupdates/

EXPLORE DERWENT WORLD PATENTS INDEX IN STN ANAVIST, VERSION 2.0: http://www.stn-international.com/archive/presentations/DWPIAnaVist2 0710.pdf

>>> XML document distribution format now available.

See HELP XMLDOC <<<

'BIX' IS DEFAULT SEARCH FIELD FOR 'WPIX' FILE

=> d stat que L43

L26 104 SEA FILE=ZCAPLUS ABB=ON PLU=ON MASAOKA S?/AU L27 6 SEA FILE=ZCAPLUS ABB=ON PLU=ON IWAZAKI H?/AU L43 1 SEA FILE=WPIX ABB=ON PLU=ON L26 AND L27

=> file zcaplus

FILE 'ZCAPLUS' ENTERED AT 12:16:12 ON 16 NOV 2007 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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FILE COVERS 1907 - 16 Nov 2007 VOL 147 ISS 22

FILE LAST UPDATED: 15 Nov 2007 (20071115/ED)

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This file contains CAS Registry Numbers for easy and accurate substance identification.

'OBI' IS DEFAULT SEARCH FIELD FOR 'ZCAPLUS' FILE

=> s L28 or L32 or L46

L47 4 L28 OR L32 OR L46

=> dup rem L47 L43

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FILE 'WPIX' ENTERED AT 12:16:30 ON 16 NOV 2007 COPYRIGHT (C) 2007 THE THOMSON CORPORATION PROCESSING COMPLETED FOR 147

PROCESSING COMPLETED FOR L47

L48

4 DUP REM L47 L43 (1 DUPLICATE REMOVED) ANSWERS '1-4' FROM FILE ZCAPLUS

THE BOAT

=> d ibib abs hitind hitstr L48 1-4

L48 ANSWER 1 OF 4 ZCAPLUS COPYRIGHT 2007 ACS on STN DUPLICATE 1

ACCESSION NUMBER:

2005:493613 ZCAPLUS Full-text

DOCUMENT NUMBER:

143:26729

TITLE:

Process for preparing phosphonium tetraarylborate compounds for use together with transition metal

complex catalysts in carbon-carbon bond,

carbon-nitrogen bond, carbon-oxygen bond formation

reactions

INVENTOR(S): Masaoka, Shin; Iwazaki, Hideyuki

PATENT ASSIGNEE(S):

Hokko Chemical Industry Co., Ltd., Japan

PCT Int. Appl., 181 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

SOURCE:

Japanese

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PAT	CENT 1	NO.			KIN	D	DATE	•		APPL					D	ATE	
WO 2005051963			A1	20050609		WO 2004-JP17628											
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		CN,	co,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FI,	GB,	GD,
		GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	ΚP,	KR,	ΚZ,	LC,
		LK,	LR,	LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NA,	NI,
		NO,	NZ,	OM,	PG,	PH,	PL,	PT,	ŖO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SY,
		TĴ,	TM,	TN,	TR,	TT,	TZ,	UA,	UG,	US,	UZ,	VC,	VN,	YU,	ZA,	ZM,	zw
	RW:	BW,	GH,	GM,	KE,	LS,	MW,	MZ,	NA,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,
		AZ,	BY,	KG,	ΚZ,	MD,	RU,	TJ,	TM,	AT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,
•		EE,	ES,	FI,	FR,	GB,	GR,	HU,	ΙE,	IS,	IT,	LU,	MC,	NL,	PL,	PT,	RO,
		SE,	SI,	SK,	TR,	BF,	ВJ,	CF,	CG,	CI,	CM,	GΑ,	GN,	GQ,	GW,	ML,	MR,
		•	•	TD,													
EP	1688	424			A 1		2006	0809	1	EP 2	004-	8194	65		2	0041	126
				FR,													
CN	1886	411			A	;	2006	1227	(CN 2	004-	8003	4977		2	0041	126

US 2007098616

Α1

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20070503
                                            US 2006-580699
                                                                   20060525
     IN 2006DN03663
                          Α
                                20070831
                                            IN 2006-DN3663
                                                                   20060626
PRIORITY APPLN. INFO.:
                                            JP 2003-399650
                                                                A 20031128
                                            JP 2003-399651
                                                                A 20031128
                                            WO 2004-JP17628
                                                                W 20041126
OTHER SOURCE(S):
                         MARPAT 143:26729
     The title compds. R1R2R3PH.BAr4 (I) [R1 = primary, secondary, or tertiary
     alkyl, cycloalkyl; R2 = H, primary, secondary, or tertiary alkyl, etc.; R3 =
     H, aryl, etc.; Ar = aryl] are prepared by reaction of R1R2R3P [R1 - R3 = as
     defined above] with HCl or sulfuric acid, followed by reaction with
     tetraarylborate M.BAr4 [M = Na, etc.; Ar = aryl]. I can be handled under air.
     Thus, treatment of a solution of tri-tert-butylphosphine in heptane with HCl,
     followed by reaction with a solution of sodium tetraphenylborate in water,
     gave tri-tert-butylphosphonium tetraphenylborate (II) in 87 mol% yield. II
     0.084 g was weighed under air and was added to a flask containing
     palladium(II) chloride 0.014 g, triethylamine 0.0194 g, and THF 5.5 mL; the
     resulting mixture was stirred at 21°C for 30 min under argon; 4-bromotoluene
     1.368 g was added; and the resulting mixture was stirred at 21°C for 30 min;
     2.2 M solution of phenylmagnesium chloride in THF 4 mL was added dropwise at
     21°C over 10 min; and the resulting mixture was stirred at 21°C for 2 h to
     give 4-methylbiphenyl in 87 mol% yield.
     ICM C07F009-54
IC
     ICS C07F005-02; C07B037-02; B01J031-24; C07F015-00
     29-7 (Organometallic and Organometalloidal Compounds)
CC
     Section cross-reference(s): 21, 25
IT
     20573-48-2P
                   131322-08-2P
                                  155234-93-8P 853073-44-6P
     853073-45-7P 853073-46-8P 853073-47-9P
     853073-48-0P 853073-50-4P 853073-51-5P
     853073-53-7P 853073-54-8P 853073-55-9P
     853073-56-0P 853073-57-1P 853073-59-3P
     853073-61-7P 853073-62-8P 853073-63-9P
     853073-64-0P 853073-65-1P 853073-66-2P
     RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation);
     USES (Uses)
        (process for preparing phosphonium tetraarylborate compds. for use
        together with transition metal complex catalysts in carbon-carbon bond,
        carbon-nitrogen bond, carbon-oxygen bond formation reactions)
IT
     853073-44-6P 853073-45-7P 853073-46-8P
     853073-47-9P 853073-48-0P 853073-50-4P
     853073-51-5P 853073-53-7P 853073-54-8P
     853073-55-9P 853073-56-0P 853073-57-1P
     853073-59-3P 853073-61-7P 853073-62-8P
     853073-63-9P 853073-64-0P 853073-65-1P
     853073-66-2P
     RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation);
     USES (Uses)
        (process for preparing phosphonium tetraarylborate compds. for use
        together with transition metal complex catalysts in carbon-carbon bond,
        carbon-nitrogen bond, carbon-oxygen bond formation reactions)
RN
     853073-44-6 ZCAPLUS
CN
     Borate(1-), tetraphenyl-, hydrogen, compd. with bis(1,1-
     dimethylethyl) methylphosphine (1:1) (9CI) (CA INDEX NAME)
     CM
          1
     CRN
         33906-65-9
         C24 H20 B . H
     CMF
     CCI CCS
```

CM 2

CRN 6002-40-0 CMF C9 H21 P

RN 853073-45-7 ZCAPLUS

CN Borate(1-), tetrakis(4-methylphenyl)-, hydrogen, compd. with bis(1,1-dimethylethyl)methylphosphine(1:1)(9CI)(CA INDEX NAME)

CM 1

CRN 78802-92-3 CMF C28 H28 B . H CCI CCS

Me $C = \frac{1}{3} + \overline{C}$ Me MeMe Me

● H +

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10/580699
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CM 2

CRN 6002-40-0 CMF C9 H21 P

Me L t-Bu—P—Bu-t

RN 853073-46-8 ZCAPLUS

CN Borate(1-), tetrakis(4-methylphenyl)-, hydrogen, compd. with tris(1,1-dimethylethyl)phosphine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 78802-92-3 CMF C28 H28 B . H

CCI CCS

Me
$$c = \frac{1}{1}$$
 $c = \frac{1}{1}$ $c = \frac{1}{1}$

● H+

CM 2

CRN 13716-12-6 CMF C12 H27 P

t-Bu t-Bu-P-Bu-t

RN 853073-47-9 ZCAPLUS

CN Borate(1-), tetraphenyl-, hydrogen, compd. with bis(1,1-dimethylethyl)ethylphosphine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 33906-65-9 CMF C24 H20 B . H CCI CCS

● H+

CM 2

CRN 25032-48-8 CMF C10 H23 P

RN 853073-48-0 ZCAPLUS

CN Borate(1-), tetraphenyl-, hydrogen, compd. with butylbis(1,1-dimethylethyl)phosphine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 33906-65-9 CMF C24 H20 B . H CCI CCS

H+

CM 2

CRN 29949-72-2 CMF C12 H27 P

t-Bu t-Bu-P-Bu-n

RN 853073-50-4 ZCAPLUS

CN Borate(1-), tetraphenyl-, hydrogen, compd. with bis(1,1-dimethylethyl)(1-methylpropyl)phosphine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 853073-49-1 CMF C12 H27 P

P(Bu-t)₂ Me-CH-Et

CM 2

CRN 33906-65-9 CMF C24 H20 B . H CCI CCS

● H⁺

RN 853073-51-5 ZCAPLUS

CN Borate(1-), tetraphenyl-, hydrogen, compd. with cyclohexylbis(1,1-dimethylethyl)phosphine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 436865-11-1 CMF C14 H29 P

CM 2

CRN 33906-65-9 CMF C24 H20 B . H

CCI CCS

● H+

RN 853073-53-7 ZCAPLUS

CN Borate(1-), tetraphenyl-, hydrogen, compd. with bis(1,1-dimethylethyl)octylphosphine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 853073-52-6 CMF C16 H35 P

Me- (CH2)7-P(Bu-t)2

CM 2

CRN 33906-65-9 CMF C24 H20 B . H

CCI CCS

● H+

RN 853073-54-8 ZCAPLUS

CN Borate(1-), tetraphenyl-, hydrogen, compd. with bis(1,1-dimethylethyl)phenylphosphine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 33906-65-9 CMF C24 H20 B . H

CCI CCS

● H+

CM 2

CRN 32673-25-9 CMF C14 H23 P

Ph t-Bu-P-Bu-t

RN 853073-55-9 ZCAPLUS

CN Borate(1-), tetraphenyl-, hydrogen, compd. with [1,1'-biphenyl]-2-ylbis(1,1-dimethylethyl)phosphine (1:1) (9CI) (CA INDEX NAME)

```
10/580699
```

CM

1

CRN 224311-51-7 CMF C20 H27 P

CM 2

CRN 33906-65-9 CMF C24 H20 B . H

CCI CCS

● H+

RN 853073-56-0 ZCAPLUS

CN Borate(1-), tetraphenyl-, hydrogen, compd. with bis(1,1-dimethylethyl)-1-naphthalenylphosphine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 200352-94-9 CMF C18 H25 P

CM 2

CRN 33906-65-9 CMF C24 H20 B . H CCI CCS

● H+

RN 853073-57-1 ZCAPLUS
CN Borate(1-), tetraphenyl-, hydrogen, compd. with bis(1,1-

dimethylethyl) (phenylmethyl) phosphine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 33906-65-9

CMF C24 H20 B . H

CCI CCS

● H+

· CM 2

CRN 27286-19-7 CMF C15 H25 P

(t-Bu)2P-CH2-Ph

RN 853073-59-3 ZCAPLUS

CN Borate(1-), tetraphenyl-, hydrogen, compd. with bis(1,1-dimethylethyl)[(4-

ethenylphenyl)methyl]phosphine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 853073-58-2 CMF C17 H27 P

CM 2

CRN 33906-65-9 CMF C24 H20 B . H

CCI CCS

● H+

RN 853073-61-7 ZCAPLUS

CN Borate(1-), tetraphenyl-, hydrogen, compd. with bis(1,1-dimethylethyl)ethenylphosphine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 853073-60-6 CMF C10 H21 P

(t-Bu)2P-CH-CH2

CM 2

CRN 33906-65-9 CMF C24 H20 B . H

CCI CCS

● H+

RN 853073-62-8 ZCAPLUS

CN Borate(1-), tetraphenyl-, hydrogen, compd. with bis(1,1-dimethylethyl)-2-propenylphosphine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 62269-82-3 CMF C11 H23 P

(t-Bu)2P-CH2-CH-CH2

CM 2

CRN 33906-65-9 CMF C24 H20 B . H CCI CCS

● H+

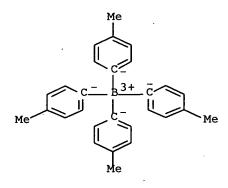
RN 853073-63-9 ZCAPLUS

CN Borate(1-), tetrakis(4-methylphenyl)-, hydrogen, compd. with tricyclohexylphosphine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 78802-92-3 CMF C28 H28 B . H

CCI CCS



● H+

CM 2

CRN 2622-14-2 CMF C18 H33 P

RN 853073-64-0 ZCAPLUS

CN Borate(1-), tetraphenyl-, hydrogen, compd. with tris(1-methylethyl)phosphine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 33906-65-9 CMF C24 H20 B . H

CCI CCS

CM 2

CRN 6476-36-4 CMF C9 H21 P

RN 853073-65-1 ZCAPLUS

Borate(1-), tetraphenyl-, hydrogen, compd. with tricyclopentylphosphine (1:1) (9CI) (CA INDEX NAME) CN

CM 1

CRN 33906-65-9 CMF C24 H20 B . H

CCI CCS

CM 2

CRN 7650-88-6

CMF C15 H27 P

RN 853073-66-2 ZCAPLUS

CN Borate(1-), tetraphenyl-, hydrogen, compd. with butyldicyclohexylphosphine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 72617-31-3 CMF C16 H31 P

CM 2

CRN 33906-65-9 CMF C24 H20 B . H CCI CCS

● H+

REFERENCE COUNT:

4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L48 ANSWER 2 OF 4 ZCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

2006:733442 ZCAPLUS Full-text

DOCUMENT NUMBER:

145:190657

TITLE:

Polyether silicone-containing aqueous antifouling

compositions, their coatings, and fish nets coated

with them

INVENTOR(S):

Masaoka, Shiqeru

PATENT ASSIGNEE(S):

Chugoku Marine Paints, Ltd., Japan

SOURCE:

Jpn. Kokai Tokkyo Koho, 19 pp.

CODEN: JKXXAF

DOCUMENT TYPE:

Patent

LANGUAGE:

Japanese

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE **_____** -----JP 2006193731 Α 20060727 JP 2005-360241 20051214 PRIORITY APPLN. INFO.: JP 2004-366299 A 20041217

The compns. contain polyether silicones and no substantial organic solvents. A mixture of Poiz 530 [poly(carboxylic acid)-based high-mol. surfactant], Adekanol UH 752 (polyether urethane viscosity regulator), and H2O was mixed with TOC 3204 [bis(dimethyldithiocarbamoyl)zinc ethylenebis(dithiocarbamate)], Newcoat TS 100 (acrylic emulsion), and KF 6016 (polyether silicone) to give a composition, which was applied to a polyethylene knotless net to give a coating showing good antifouling property for 6 mo.

42-7 (Coatings, Inks, and Related Products) CC

Section cross-reference(s): 5

97-77-8, Tetraethylthiuram disulfide 1317-39-1, Cuprous oxide, uses IT 7440-50-8, Copper, uses 13463-41-7, Zinc pyrithione 17648-71-4, N, N'-Dimethyl-N'-phenyl-(N-fluorodichloromethylthio) sulfamide 56746-18-0, 2,3-Dichloro-N-(2',6'-diethylphenyl)maleimide 64359-81-5. 4,5-Dichloro-2-octyl-4-isothiazolin-3-one 64440-88-6, TOC 3204 106916-69-2 107065-10-1, Triphenyl (octadecylamine) **boron** 117659-55-9, 2,3-Dichloro-N-(2'-ethyl-6'-methylphenyl)maleimide 154592-20-8, Copper pyrithione 180128-56-7, Chloromethyl octyl disulfide 250578-38-2, Triphenyl[3-(2-ethylhexyloxy)propylamine]boron 459424-07-8, Asankadou NC 301 900534-06-7, Diphenylmethylisopropylamineb oron

RL: BUU (Biological use, unclassified); MOA (Modifier or additive use); TEM (Technical or engineered material use); BIOL (Biological study); USES

(antifouling agent; aqueous antifouling coatings containing polyether

for fish nets)

L48 ANSWER 3 OF 4 ZCAPLUS COPYRIGHT 2007 ACS on STN ACCESSION NUMBER: 2002:575117 ZCAPLUS Full-text

DOCUMENT NUMBER:

TITLE:

137:125533 Polymerization of olefinic compounds by polymerization

catalyst complexes containing phosphino, amino, or

imino groups

INVENTOR(S):

Brookhart, Maurice S.; Kunitsky, Keith; Malinoski, Jon M.; Wang, Lin; Wang, Yin; Liu, Weijun; Johnson, Lynda

Kaye; Kreutzer, Kristina A.; Ittel, Steven Dale

PATENT ASSIGNEE(S):

E. I. Du Pont de Nemours & Co., USA

SOURCE:

PCT Int. Appl., 77 pp. CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.

KIND DATE

APPLICATION NO.

DATE

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WO 2002059165
                          A2
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                                                                    20020125
     WO 2002059165
                          A3
                                20030522
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             LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
             PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ,
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     US 2005043496
                          A1
                                20050224
                                            US 2004-943199
                                                                    20040916
                                            US 2001-264537P
PRIORITY APPLN. INFO.:
                                                                 P 20010126
                                            US 2001-294794P
                                                                 P 20010531
                                            US 2001-871099
                                                                 A 20010531
                                            US 2000-208087P
                                                                 P 20000531
                                            US 2000-211601P
                                                                 P 20000615
                                            US 2000-214036P
                                                                 P 20000623
                                            US 2002-57090
                                                                 A3 20020125
                                            WO 2002-US3088
                                                                 W 20020125
OTHER SOURCE(S):
                         MARPAT 137:125533
AB
     Certain complexes containing ligands having a phosphino group, amino group, or
     an imino group, and a second functional group such as amide, ester, or ketone,
     when complexed to transition metals, catalyze the (co)polymerization of
     olefinic compds. such as ethylene, \alpha-olefins and/or acrylates. A newly
     recognized class of ligands for making copolymer containing polar monomers
     using late transition metal complexes is described.
IC
     ICM C08F010-00
CC
     35-3 (Chemistry of Synthetic High Polymers)
ΙT
     220313-59-7P
                    378797-06-9P
                                   378797-08-1P
                                                   378797-10-5P
                                                                  378797-14-9P
     378797-16-1P
                    378797-18-3P
                                   444107-56-6P
                                                   444107-61-3P
                                                                  444107-64-6P
     444107-66-8P
                    444107-69-1P
                                   444107-72-6P
                                                   444107-74-8P
                                                                  444107-77-1P
     444107-88-4P
                    444107-90-8P
                                   444107-92-0P
                                                   444107-95-3P
                                                                  444107-96-4P
     444107-98-6P
                    444108-00-3P
                                   444108-02-5P
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                                                                  444108-06-9P
     444108-07-0P
                    444108-09-2P
                                   444108-18-3P
                                                   444108-21-8P
     444108-24-1P
                    444108-26-3P
     RL: CAT (Catalyst use); IMF (Industrial manufacture); PREP (Preparation);
     USES (Uses)
        (catalyst; polymerization of olefinic compds. by polymerization catalyst
        containing phosphino, amino, or imino groups)
IT
     960-71-4, Triphenylboron 1109-15-5, Tris(pentafluorophenyl)boron
     RL: CAT (Catalyst use); USES (Uses)
        (cocatalyst; polymerization of olefinic compds. by polymerization catalyst
complexes
        containing phosphino, amino, or imino groups)
```

IT 444108-07-0P

RL: CAT (Catalyst use); IMF (Industrial manufacture); PREP (Preparation); USES (Uses)

containing phosphino, amino, or imino groups)

RN 444108-07-0 ZCAPLUS

CN Nickel(1+), [1-[bis(1,1-dimethylethyl)phosphino-κP]-3-[bis(1,1-dimethylethyl)phosphino]-1,3-dihydro-2H-inden-2-one-κO][(1,2,3-η)-2-(methoxycarbonyl)-2-propenyl]-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (9CI). (CA INDEX NAME)

CM 1

CRN 378793-54-5

CMF C30 H49 Ni O3 P2

CCI CCS

PAGE 1-A

$$t-Bu$$
 $t-Bu$
 $t-Bu$

PAGE 2-A

Ŋ

CM 2

CRN 79230-20-9 CMF C32 H12 B F24

CCI CCS

L48 ANSWER 4 OF 4 ZCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

1999:394727 ZCAPLUS Full-text

DOCUMENT NUMBER:

131:60118

TITLE:

Antifouling coating compositions, their films, and

their use in fouling control of ships

INVENTOR(S):

Masaoka, Shigeru; Yamato, Masafumi

PATENT ASSIGNEE(S):

Chugoku Marine Paints, Ltd., Japan

SOURCE:

Jpn. Kokai Tokkyo Koho, 9 pp.

CODEN: JKXXAF

DOCUMENT TYPE:

Patent

LANGUAGE:

Japanese

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 11166136	Α	19990622	JP 1997-333143	19971203
PRIORITY APPLN. INFO.:			JP 1997-333143	19971203
OTHER SOURCE(S):	MARPAT	131:60118		

The compns., useful for fouling control of outer surfaces of ships, contain 2-20% Ph3B.NH2R1 (R1 = C3-30 alkyl), Cu compds., and film-forming components. Thus, WW Rosin 11, Laroflex MP 15 (vinyl chloride-vinyl iso-Bu ether copolymer) 7, E 028-90X (epoxy resin) 0.3, Ti White 5, ZnO 6, Cu2O 35, Ph3B-dodecylamine complex 10, Disparlon 630-20X (fatty amide wax) 3.5, PhMe 4, and xylene 18.2 parts were mixed to give a coating showing almost complete prevention of marine organism adhesion, excellent curability, and no cracking after soaking in seawater for 12 mo.

IC ICM C09D005-16

ICS B63B059-04; C09D007-12

CC 42-10 (Coatings, Inks, and Related Products) Section cross-reference(s): 5

ST antifouling coating phenylboron amine complex copper; ship fouling control coating **boron** complex; vinyl polymer coating antifouling **boron** complex

=> file registry
FILE 'REGISTRY' ENTERED AT 12:17:47 ON 16 NOV 2007
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STRUCTURE FILE UPDATES: 15 NOV 2007 HIGHEST RN 953991-83-8 DICTIONARY FILE UPDATES: 15 NOV 2007 HIGHEST RN 953991-83-8

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=> file zcaplus FILE 'ZCAPLUS' ENTERED AT 12:17:51 ON 16 NOV 2007 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2007 AMERICAN CHEMICAL SOCIETY (ACS)

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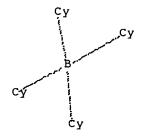
FILE COVERS 1907 - 16 Nov 2007 VOL 147 ISS 22 FILE LAST UPDATED: 15 Nov 2007 (20071115/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

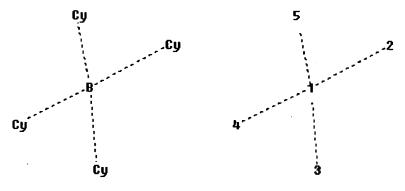
This file contains CAS Registry Numbers for easy and accurate substance identification.

'OBI' IS DEFAULT SEARCH FIELD FOR 'ZCAPLUS' FILE

=> d stat que L25 L2 STR



Structure attributes must be viewed using STN Express query preparation: Uploading L2.str



chain nodes:
1 2 3 4 5
chain bonds:
1-2 1-3 1-4 1-5
exact/norm bonds:
1-2 1-3 1-4 1-5

Match level:

1:CLASS 2:Atom 3:Atom 4:Atom 5:Atom

Generic attributes :

2:

Saturation : Unsaturated

3:

Saturation : Unsaturated

4:

Saturation : Unsaturated

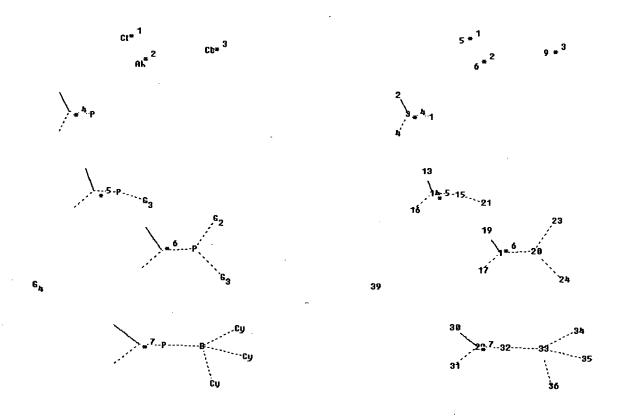
5:

Saturation : Unsaturated

L5 25294 SEA FILE=REGISTRY SSS FUL L2 L8 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation: Uploading L8.str



chain nodes:
1 5 6 9 15 20 21 23 24 32 33 34 35 36 39
ring/chain nodes:
2 3 4 13 14 16 17 18 19 29 30 31
chain bonds:

1-3 14-15 15-21 18-20 20-23 20-24 29-32 32-33 33-34 33-35 33-36 ring/chain bonds :

2-3 3-4 13-14 14-16 17-18 18-19 29-31 29-30 exact/norm bonds:

1-3 3-4 14-15 14-16 15-21 17-18 18-20 20-23 20-24 29-31 29-32 32-33 33-

33-35 33-36 exact bonds:

2-3 13-14 18-19 29-30

G2:[*1],[*2]

G3:[*1],[*2],[*3]

G4:[*4],[*5],[*6],[*7]

Connectivity:

1:1 E exact RC ring/chain 15:2 E exact RC ring/chain 20:3 E exact RC ring/chain

Match level :

1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:Atom 6:CLASS 9:Atom 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS 21:CLASS 23:CLASS

24:CLASS 29:CLASS

30:CLASS 31:CLASS 32:CLASS 33:CLASS 34:Atom 35:Atom 36:Atom 39:CLASS

Generic attributes :

5:

Saturation : Saturated

9:

Saturation : Unsaturated

34:

Saturation : Unsaturated

35:

Saturation : Unsaturated

36:

Saturation : Unsaturated

L10 L11 (47 SEA FILE=REGISTRY SUB=L5 SSS FUL L8 129) SEA FILE=REGISTRY ABB=ON PLU=ON (100-42-5/BI OR 100-47-0/BI OR 100-59-4/BI OR 10273-89-9/BI OR 105-56-6/BI OR 106-38-7/BI OR 106-99-0/BI OR 1066-54-2/BI OR 107-05-1/BI OR 107-15-3/BI OR 1078-71-3/BI OR 1078-71-3/BI OR 108-86-1/BI OR 107-05-1/BI OR 109-09-1/BI OR 109-69-3/BI OR 110-86-1/BI OR 111-85-3/BI OR 1122-91-4/BI OR 113279-72-4/BI OR 115-19-5/BI OR 122-39-4/BI OR 123-54-6/BI OR 113227-08-2/BI OR 13597-73-4/BI OR 122-39-4/BI OR 123-54-6/BI OR 131322-08-2/BI OR 13597-73-4/BI OR 13716-10-4/BI OR 13716-12-6/BI OR 143-66-8/BI OR 15181-07-4/BI OR 155534-93-8/BI OR 15738-23-5/BI OR 1592-20-7/BI OR 16419-60-6/BI OR 16523-54-9/BI OR 200352-94-9/BI OR 2042-85-5/BI OR 20488-42-0/BI OR 20573-48-2/BI OR 224311-51-7/BI OR 2350-89-2/B I OR 25032-48-8/BI OR 2622-14-2/BI OR 2920-38-9/BI OR 29949-72-2/BI OR 2996-92-1/BI OR 29965-97-7/BI OR 32673-25-9/BI OR 3375-31-3/BI OR 356518-17-7/BI OR 42092-01-3/BI OR 4553-07-5/BI OR 460-00-4/BI OR 501-65-5/BI OR 50704-04-6/BI OR 51364-51-3/B I OR 536-74-3/BI OR 56512-48-2/BI OR 56522-08-8/BI OR 5720-05-8/B I OR 542-92-7/BI OR 603-35-0/BI OR 623-03-0/BI OR 629-04-9/BI OR 629-06-1/BI OR 603-35-0/BI OR 623-03-0/BI OR 643-58-3/BI OR 629-04-9/BI OR 6476-36-4/BI OR 6738-23-4/BI OR 643-58-3/BI OR 7439-96-5/BI OR 7440-02-0/BI OR 6738-23-4/BI OR 7439-95-4/BI OR 7440-16-6/BI OR 7440-02-0/BI OR 7440-05-3/BI OR 7440-06-4/BI OR 7440-06-4/BI OR 7440-01-8/BI OR 7440-08-3/BI OR 7440-06-4/BI OR 7440-16-6/BI OR 7440-18-8/BI OR 7646-93-9/BI OR 7440-06-4/BI OR 75501-4/BI OR 7647-10-1/BI OR 7646-93-9/BI OR 7440-06-4/BI OR 75501-4/BI OR 7647-10-1/BI OR 7646-93-9/BI OR 7646-85-7/BI OR 753073-46-0/BI OR 853073-46-0/BI OR 853073-46-0/BI OR 853073-54-7/BI OR 853073-54-7/BI OR 853073-54-7/BI OR 853073-55-7/BI OR 85
L12 (-8/BI OR 853073-55-9/BI OR 85
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L14	22 SEA FILE=REGISTRY ABB=ON PLU=ON L12 AND L13
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OR 155234-93-8/BI OR 15738-23-5/BI OR 1592-20-7/BI OR 16419-60-6/BI OR 16523-54-9/BI OR 200352-94-9/BI OR 2042-85-5/BI OR 20488-42-0/BI OR 20573-48-2/BI OR 224311-51-7/BI OR 2350-89-2/B I OR 25032-48-8/BI OR 2622-14-2/BI OR 2920-38-9/BI OR 29949-72-2/BI OR 2996-92-1/BI OR 29965-97-7/BI OR 32673-25-9/BI OR 3375-31-3/BI OR 356518-17-7/BI OR 42092-01-3/BI OR 4553-07-5/BI OR 460-00-4/BI OR 501-65-5/BI OR 50704-04-6/BI OR 51364-51-3/B I OR 536-74-3/BI OR 538-58-9/BI OR 541-16-2/BI OR 542-18-7/BI OR 542-92-7/BI OR 56512-48-2/BI OR 56522-08-8/BI OR 5720-05-8/B I OR 586-77-6/BI OR 6002-40-0/BI OR 603-34-9/BI OR 603-35-0/BI OR 623-03-0/BI OR 629-04-9/BI OR 629-06-1/BI OR 629-20-9/BI OR 64-19-7/BI OR 643-58-3/BI OR 644-08-6/BI OR 6476-36-4/BI OR 6738-23-4/BI OR 6781-98-2/BI OR 72617-31-3/BI OR 74-85-1/BI OR 7439-89-6/BI OR 7439-95-4/BI OR 7439-96-5/BI OR 7440-02-0/BI OR 7440-05-3/BI OR 7440-06-4/BI OR 7440-16-6/BI OR 7440-18-8/BI OR 7440-48-4/BI OR 7459-73-6/BI OR 75-01-4/BI OR 75-05-8/BI OR 76-05-1/BI OR 7646-85-7/BI OR 7647-01-0/BI OR 7647-10-1/BI OR 7664-93-9/BI OR 77123-57-0/BI OR 7719-12-2/BI OR 78-86-4/BI OR 80-62-6/BI OR 81233-93-4/BI OR 853073-44-6/BI OR 853073-45-7 /BI OR 853073-46-8/BI OR 853073-47-9/BI OR 853073-48-0/BI OR 853073-50-4/BI OR 853073-51-5/BI OR 853073-53-7/BI OR 853073-54 -8/BI OR 853073-55-9/BI OR 85

		-,	
L16	(38) SEA FILE=REGISTRY ABB=ON PLU=ON L15 AND P/ELS	
L17	(27) SEA FILE=REGISTRY ABB=ON PLU=ON L15 AND B/ELS	
L18	(22) SEA FILE=REGISTRY ABB=ON PLU=ON L16 AND L17	
L19	(3) SEA FILE=REGISTRY ABB=ON PLU=ON (20573-48-2/BI OR 131322-08	-2
		/BI OR 155234-93-8/BI)	
L20		19 SEA FILE=REGISTRY ABB=ON PLU=ON L18 NOT L19	
L21		21 SEA FILE=REGISTRY ABB=ON PLU=ON L10 AND L14	
L23		2 SEA FILE=REGISTRY ABB=ON PLU=ON L21 NOT L20	
L24		45 SEA FILE=REGISTRY ABB=ON PLU=ON L10 NOT L23	
L25		18 SEA FILE=ZCAPLUS ABB=ON PLU=ON L24	

=> s L25 not L48

L49 4 S L48

L50 16 L25 NOT L49

=> file babs

FILE 'BABS' ENTERED AT 12:18:50 ON 16 NOV 2007 .
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FILE LAST UPDATED:

25 JUN 2007

<20070625/UP>

FILE COVERS 1980 TO DATE.

=> d stat que L39

L39 4 SEA FILE=BABS ABB=ON PLU=ON (6281441/BABSAN OR 6594776/BABSAN OR 6580383/BABSAN OR 6432734/BABSAN)

=> file beilstein

FILE 'BEILSTEIN' ENTERED AT 12:19:02 ON 16 NOV 2007 COPYRIGHT (c) 2007 Beilstein-Institut zur Foerderung der Chemischen Wissenschaften licensed to Beilstein GmbH and MDL Information Systems GmbH

FILE LAST UPDATED ON September 26, 2007

FILE COVERS 1771 TO 2007.

*** FILE CONTAINS 10.119,480 SUBSTANCES ***

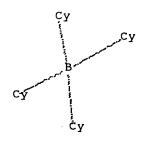
>>>PLEASE NOTE: Reaction Data and substance data are stored in separate documents and can not be searched together in one query. Reaction data for BEILSTEIN compounds may be displayed immediately with the display codes PRE (preparations) and REA (reactions). A substance answer set retrieved after the search for a chemical name, a compounds with available reaction information by combining with PRE/FA, REA/FA or more generally with RX/FA. The BEILSTEIN Registry Number (BRN) is the link between a BEILSTEIN compound and belonging reactions. For mo detailed reaction searches BRNs can be searched as reaction partner BRNs Reactant BRN (RX.RBRN) or Product BRN (RX.PBRN).<<<

>>> FOR SEARCHING PREPARATIONS SEE HELP PRE <<<

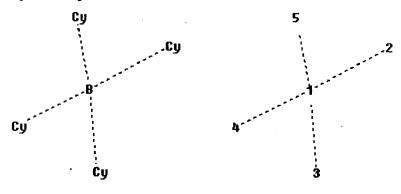
NEW

- * PATENT NUMBERS (PN) AND BABS ACCESSION NUMBERS (BABSAN) CAN NOW BE SEARCHED, SELECTED AND TRANSFERRED.
- * NEW DISPLAY FORMATS ALLREF, ALLP AND BABSAN SHOW ALL REFERENCES, ALL PATENT REFERENCES, OR ALL BABS ACCESSION NUMBERS FOR A COMPOUND AT A GLANCE.

=> d stat que L41 L2 STR



Structure attributes must be viewed using STN Express query preparation: Uploading L2.str



chain nodes:
1 2 3 4 5
chain bonds:
1-2 1-3 1-4 1-5
exact/norm bonds:
1-2 1-3 1-4 1-5

Match level:

1:CLASS 2:Atom 3:Atom 4:Atom 5:Atom

Generic attributes :

2:

Saturation : Unsaturated

3:

Saturation : Unsaturated

4:

Saturation : Unsaturated

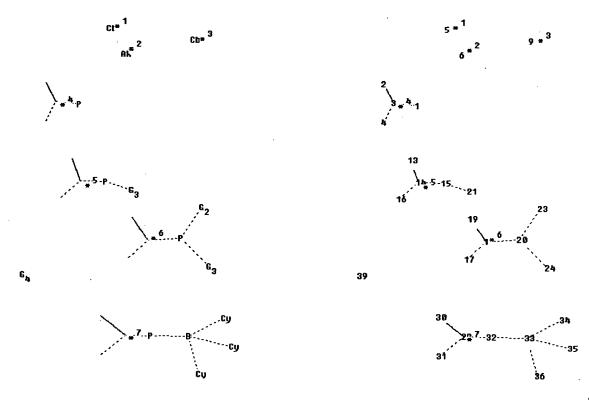
5:

Saturation : Unsaturated

L8 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation: Uploading L8.str



```
chain nodes :
1 5 6 9 15 20 21 23 24 32 33 34 35 36 39
ring/chain nodes :
2 3 4 13 14 16 17 18 19 29 30 31
chain bonds :
1-3 14-15 15-21 18-20 20-23 20-24 29-32 32-33 33-34 33-35 33-36
ring/chain bonds :
2-3 3-4 13-14 14-16 17-18 18-19 29-31 29-30
exact/norm bonds :
1-3 3-4 14-15 14-16 15-21 17-18 18-20 20-23 20-24 29-31 29-32 32-33 33-
33-35 33-36
exact bonds :
2-3 13-14 18-19 29-30
G2:[*1],[*2]
G3: [*1], [*2], [*3]
G4: [*4], [*5], [*6], [*7]
Connectivity:
1:1 E exact RC ring/chain 15:2 E exact RC ring/chain 20:3 E exact RC ring/chain
Match level:
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:Atom 6:CLASS 9:Atom 13:CLASS 14:CLASS
15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS 21:CLASS 23:CLASS
24:CLASS 29:CLASS
30:CLASS 31:CLASS 32:CLASS 33:CLASS 34:Atom 35:Atom 36:Atom 39:CLASS
Generic attributes :
5:
Saturation
            : Saturated
9:
Saturation
            : Unsaturated
34:
              : Unsaturated
Saturation
35:
Saturation
                   : Unsaturated
36:
Saturation
                   : Unsaturated
         2084 SEA FILE=BEILSTEIN SSS FIII. 1.2
```

ГЭЭ	2004	SEA	CIPE-DEIT21FIN	222 LOT	١Z			
L37	16	SEA	FILE=BEILSTEIN	SUB=L35	SSS FUL	T8		
L38	9	SEA	FILE=BEILSTEIN	ABB=ON	PLU=ON	L37	AND	BABSAN/FA
L41	7	SEA	FILE=BEILSTEIN	ABB=ON	PLU=ON	L37	NOT	L38

=> dup rem L50 L39 L41
DUPLICATE IS NOT AVAILABLE IN 'BEILSTEIN'.
ANSWERS FROM THESE FILES WILL BE CONSIDERED UNIQUE
FILE 'ZCAPLUS' ENTERED AT 12:19:19 ON 16 NOV 2007
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PROCESSING COMPLETED FOR L50 PROCESSING COMPLETED FOR L39 PROCESSING COMPLETED FOR L41

L51 24 DUP REM L50 L39 L41 (3 DUPLICATES REMOVED)

ANSWERS '1-16' FROM FILE ZCAPLUS

ANSWER '17' FROM FILE BABS

ANSWERS '18-24' FROM FILE BEILSTEIN

=> d ibib abs hitstr L51 1-16; d iall L51 17; d ide allref L51 18-24

L51 ANSWER 1 OF 24 ZCAPLUS COPYRIGHT 2007 ACS on STN DUPLICATE 1

ACCESSION NUMBER: DOCUMENT NUMBER:

2006:433685 ZCAPLUS Full-text 145:136705

TITLE:

An acidity scale of phosphonium tetraphenylborate

salts and ruthenium dihydrogen complexes in

dichloromethane

AUTHOR(S):

Li, Tianshu; Lough, Alan J.; Zuccaccia, Cristiano;

Macchioni, Alceo; Morris, Robert H.

CORPORATE SOURCE:

Department of Chemistry, University of Toronto,

Toronto, ON, M5S 3H6, Can.

SOURCE:

Canadian Journal of Chemistry (2006), 84(2), 164-175

CODEN: CJCHAG; ISSN: 0008-4042

PUBLISHER:

National Research Council of Canada

DOCUMENT TYPE:

Journal

LANGUAGE: English AB

Equilibrium consts. (KDM) for reactions between acids and bases of the title compds. in CD2C12 (DM) were determined by 31P and 1H NMR spectroscopy at room temperature [HPCy3]BPh4 and [HPCy3]BF4, with pKDM assigned by literature convention to 9.7, were used as the anchor compds. for the pKDM detns. A continuous scale of pKDM values covering the range 9.7 to 5.7 is created with the acidic compds. [HPR3]BPh4. Those acids with pKDM >6 are stable, while those with more acidic cations HPR3+ protonate BPh4- to produce R3PBPh3 and benzene. The literature pKTHF values reported for [HPBu2Ph]BPh4, [HPMePh2]BPh4, and [HPEtPh2]BPh4 are questionable because of this protonation reaction. NOE and PGSE 1H NMR techniques were used to show that [HPCy2Ph]BPh4 in DM exists as ion pairs and higher aggregates up to quadrupoles at the concns. used in the acid-base studies. The new dihydrogen complexes [Ru(H2)Cl(PPh3)2(dach)]BF4(dach = (1R,2R)-(-)-diaminocyclohexane) and $[Ru(H2)Cl\{tmeP2(NH)2\}]BF4$ (tmeP2(NH)2 = PPh2C6H4CH2NHCMe2CMe2NHCH2C6H4PPh2)were prepared by reaction of RuHCl(PPh3)2(dach) and RuHCl{tmeP2(NH)2} with HBF4. Their crystal structures are reported, and the pKDM values of their BPh4- salts are 8.6 and 6.9, resp.

IT 853073-54-8 897015-21-3

RL: PRP (Properties)

(acidity scale from equilibrium consts. of phosphonium tetraphenylborate salts and ruthenium dihydrogen complexes in dichloromethane)

853073-54-8 ZCAPLUS RN

CN Borate(1-), tetraphenyl-, hydrogen, compd. with bis(1,1dimethylethyl)phenylphosphine (1:1) (9CI) (CA INDEX NAME)

CM 1 CRN 33906-65-9 CMF C24 H20 B . H CCI CCS

⊕ H +

CM 2

CRN 32673-25-9 CMF C14 H23 P

RN 897015-21-3 ZCAPLUS

CN Borate(1-), tetraphenyl-, hydrogen, compd. with dicyclohexylphenylphosphine (1:1) (9CI) (CA INDEX NAME)

CM 1

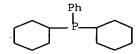
CRN 33906-65-9 CMF C24 H20 B . H CCI CCS

CCI CCS

● H+

CM

CRN 6476-37-5 CMF C18 H27 P



THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS REFERENCE COUNT: 46 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L51 ANSWER 2 OF 24 ZCAPLUS COPYRIGHT 2007 ACS on STN DUPLICATE 2

2003:149747 ZCAPLUS Full-text ACCESSION NUMBER:

139:117473

DOCUMENT NUMBER:

TITLE:

SOURCE:

Sterically crowded diphosphinomethane ligands:

molecular structures, UV-photoelectron spectroscopy and a convenient general synthesis of tBu2PCH2PtBu2

and related species

AUTHOR(S): Eisentraeger, Frank; Goethlich, Alexander; Gruber,

Irene; Heiss, Helmut; Kiener, Christoph A.; Krueger, Carl; Ulrich Notheis, J.; Rominger, Frank; Scherhag, Gunter; Schultz, Madeleine; Straub, Bernd F.; Volland,

Martin A. O.; Hofmann, Peter

CORPORATE SOURCE: Organisch-Chemisches Institut der Ruprecht-Karls-

Universitaet Heidelberg, Heidelberg, D-69120, Germany

New Journal of Chemistry (2003), 27(3), 540-550

CODEN: NJCHE5; ISSN: 1144-0546

PUBLISHER: Royal Society of Chemistry DOCUMENT TYPE: Journal

LANGUAGE:

English

OTHER SOURCE(S): CASREACT 139:117473

A series of highly crowded sym. and unsym. diphosphinomethanes R2PCH2PR12, important ligands in transition metal chemical and catalysis, namely tBu2PCH2PtBu2 (dtbpm, 1), Cy2PCH2PCy2 (dcpm, 2), tBu2PCH2PCy2 (ctbpm, 3), tBu2PCH2PiPr2 (iptbpm, 4) and tBu2PCH2PPh2 (ptbpm, 5), was prepared in high yields, using a general and convenient route. Lithiation of tBu2PMe gave tBu2PCH2Li, which reacted with R12PCl (R = tBu, Cy, iPr, Ph) resulting in high yields of 1, 3-5; the same route conveniently gave diphosphine 2. These compds. are crystalline solids at room temperature, besides of 4, which is a colorless liquid Their mol. structures were determined by single crystal xray diffraction, along with that of the higher homolog of 1, tBu2CH2CH2tBu2 (dtbpe, 6). The solid-state structures of the dioxide tBu2P(0)CH2P(0)tBu2 (7), and of two phosphonium cations derived from 1, protonated [tBu2P(H)CH2PtBu2]+ (8+) and the chlorophosphonium ion [tBu2P(Cl)CH2PtBu2]+ (9+), are also described and show a distinct structural influence of the tetracoordinate P centers. The gas phase UV-photoelectron spectra of the diphosphines 1-6 were measured. Their first two ionization potentials are nearly degenerate and all are in the low energy range from 7.5 to 7.8 eV. Comparison with related mono- and bidentate phosphines demonstrates that 1-6 are excellent σ -donors towards metals, in accord with their known coordination chemical Mol. geometries and electronic structures of the diphosphines were studied by quantum chemical calcns. and are compared to experiment Unlike standard semiempirical methods (AM1, PM3, MNDO), which give rather poor min. structures and seem inadequate for such sterically crowded systems, ab initio calcns. (RHF/6-31G**) predict mol. geometries with reasonable accuracy and reflect the observed trends in exptl. ionization potentials.

IT 563539-90-2P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (crystal structure; preparation, structure and UPS of sterically crowded methylenediphosphines)

RN 563539-90-2 ZCAPLUS

CN Borate(1-), tetrakis[3,5-bis(trifluoromethyl)phenyl]-, hydrogen, compd. with methylenebis[bis(1,1-dimethylethyl)phosphine] (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 121281-53-6 CMF C32 H12 B F24 . H CCI CCS

H+

CM 2

CRN 87648-10-0 CMF C17 H38 P2

(t-Bu) 2P - CH2-P(Bu-t) 2

REFERENCE COUNT: 82 THERE ARE 82 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L51 ANSWER 3 OF 24 ZCAPLUS COPYRIGHT 2007 ACS on STN ACCESSION NUMBER: 2007:119055 ZCAPLUS Full-text

DOCUMENT NUMBER:

146:184915

TITLE:

Method of preparing phosphonium compound for cyclic

olefin polymerization

INVENTOR(S):

Yoon, Sungcheol; Won, Young-Chul; Park, Young-Whan;

Chun, Sung-Ho; Choi, Dai-Seung

PATENT ASSIGNEE(S): Lg Chem, Ltd., S. Korea SOURCE: PCT Int. Appl., 27pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent English

LANGUAGE:

• 1

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

WO 2007013759 A1 20070201 WO 2006-KR2925 2	20060725
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ,	, CA, CH,
CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI,	, GB, GD,
GE, GH, GM, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM,	, KN, KP,
KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK,	, MN, MW,
MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS,	, RU, SC,
SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA,	UG, US,
UZ, VC, VN, ZA, ZM, ZW	
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR,	, HU, IE,
IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR,	
CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG,	, BW, GH,
GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,	AZ, BY,
KG, KZ, MD, RU, TJ, TM	
KR 2007014035 A 20070131 KR 2006-69534 2	20060725
US 2007027277 A1 20070201 US 2006-492059 2	20060725
PRIORITY APPLN. INFO.: KR 2005-67830 A 2	20050726
KR 2006-69534 A 2	0060725

OTHER SOURCE(S): MARPAT 146:184915

AB Provided is a method of preparing a phosphonium compound by reacting a protic phosphonium compound represented by [(R1)P(R2)a(R2)b]HX and a salt compound Therefore, a phosphonium compound used as a cocatalyst for the preparation of a polar cyclic olefin polymer can be produced at high yield.

IT 872885-08-0P, Tricyclohexylphosphonium

tetrakis (pentafluorophenyl) borate 872885-10-4P,

Tri-tert-butylphosphonium tetrakis(pentafluorophenyl)borate

RL: CAT (Catalyst use); IMF (Industrial manufacture); PREP (Preparation); USES (Uses)

(method of preparing phosphonium compound for cyclic olefin polymerization) RN 872885-08-0 ZCAPLUS

CN Borate(1-), tetrakis(pentafluorophenyl)-, hydrogen, compd. with tricyclohexylphosphine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 118611-98-6

CMF C24 B F20 . H

CCI CCS

● H +

CM 2

CRN 2622-14-2 CMF C18 H33 P

RN 872885-10-4 ZCAPLUS

CN Borate(1-), tetrakis(pentafluorophenyl)-, hydrogen, compd. with tris(1,1-dimethylethyl)phosphine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 118611-98-6 CMF C24 B F20 . H

CCI CCS

● H +

CM 2

CRN 13716-12-6 CMF C12 H27 P

t-Bu | t-Bu-P-Bu-t

REFERENCE COUNT:

THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L51 ANSWER 4 OF 24 ACCESSION NUMBER:

ZCAPLUS COPYRIGHT 2007 ACS on STN 2007:830082 ZCAPLUS Full-text

DOCUMENT NUMBER:

147:448289

4

TITLE:

. Tuning Lewis acidity using the reactivity of

"frustrated Lewis pairs": facile formation of

phosphine-boranes and cationic phosphonium-boranes Welch, Gregory C.; Cabrera, Lourdes; Chase, Preston

AUTHOR(S):

A.; Hollink, Emily; Masuda, Jason D.; Wei, Pingrong;

Stephan, Douglas W.

CORPORATE SOURCE:

Department of Chemistry & Biochemistry, University of

Windsor, Windsor, ON, N9B3P4, Can.

SOURCE:

Dalton Transactions (2007), (31), 3407-3414

CODEN: DTARAF; ISSN: 1477-9226

PUBLISHER:

Royal Society of Chemistry

DOCUMENT TYPE:

Journal

LANGUAGE:

English

The concept of "frustrated Lewis pairs" involves donor and acceptor sites in which steric congestion precludes Lewis acid-base adduct formation. In the case of sterically demanding phosphines and boranes, this lack of self-quenching prompts nucleophilic attack at a carbon para to B followed by fluoride transfer affording zwitterionic phosphonium borates
[R3P(C6F4)BF(C6F5)2] and [R2PH(C6F4)BF(C6F5)2]. These can be easily transformed into the cationic phosphonium-boranes [R3P(C6F4)B(C6F5)2]+ and [R2PH(C6F4)B(C6F5)2]+ or the neutral phosphino-boranes R2P(C6F4)B(C6F5)2. This new reactivity provides a modular route to a family of boranes in which the

steric features about the Lewis acidic center remains constant and yet the variation in substitution provides a facile avenue for the tuning of the Lewis acidity. Employing the Gutmann-Beckett and Childs methods for determining Lewis acid strength, it is demonstrated that the cationic boranes are much more Lewis acidic than B(C6F5)3, while the acidity of the phosphine-boranes is diminished.

IT 947699-01-6P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (tuning Lewis acidity using reactivity of frustrated Lewis pairs in facile formation of phosphine boranes and cationic phosphonium boranes)

RN 947699-01-6 ZCAPLUS

CN INDEX NAME NOT YET ASSIGNED

CM 1

CRN 947699-00-5 CMF C26 H18 B F14 P

CM 2

CRN 118611-98-6 CMF C24 B F20 . H CCI CCS

$$F \qquad F \qquad F$$

$$F \qquad C \qquad F \qquad F$$

$$F \qquad F \qquad F$$

$$F \qquad F \qquad F$$

● # +

L51 ANSWER 5 OF 24 ZCAPLUS COPYRIGHT 2007 ACS on STN 2006:673982 ZCAPLUS Full-text ACCESSION NUMBER:

DOCUMENT NUMBER:

145:146211

TITLE:

Manufacture of photoreactive polymers

INVENTOR(S):

Kim, Heon; Chun, Sung-Ho; Lee, Keon-Woo; Oh,

Sung-Joon; Kim, Kyungjun; Jo, Jungho; Lee, Byung-Hyun;

Lim, Min-Young; Jeong, Hye-Won

PATENT ASSIGNEE(S): SOURCE:

LG Chem, Ltd., S. Korea PCT Int. Appl., 48 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

	PA	PATENT NO.				KIND DATE			APPLICATION NO.						DATE			
	WO	WO 2006073270			A1 20060713			WO 2006-KR39					20060105					
		W:	ΑE,	AG,	AL,	AM,	AT,	AU,	AZ,	BA,	BB,	BG,	BR,	BW,	BY,	BZ,	CA,	CH,
			CN,	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FI,	GB,	GD,
			GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	ΚM,	KN,	KP,	ΚZ,
			LC,	LK,	LR,	LS,	LT,	LU,	LV,	LY,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,
			NA,	NG,	NI,	NO,	ΝZ,	OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,
			SK,	SL,	SM,	SY,	TJ,	TM,	TN,	TR,	TT,	TZ,	UA,	ŪG,	UZ,	VC,	VN,	YU,
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			IS,	IT,	LT,	LU,	LV,	MC,	NL,	PL,	PT,	RO,	SE,	SI,	SK,	TR,	BF,	ВJ,
0			CF,	CG,	CI,	CM,	GΑ,	GN,	GQ,	GW,	ML,	MR,	NE,	SN,	TD,	TG,	BW,	GH,
			GM,	KE,	LS,	MW,	MZ,	NA,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,	ΑZ,	BY,
			KG,	ΚZ,	MD,	RU,	ТJ,	TM										
		2006				Α		2006	0710	:	KR 2	006-	1087			2	0060	104
		2006		70		A 1		2006	0720	1	US 2	006-	3254	14		2	0060	105
	EP	1833				A1		2007			EP 2						0060	
		R:	AT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,	EE,	ES,	FI,	FR,	GB,	GR,	HU,	IE,
						LT,	LU,	LV,	MC,	NL,	PL,	PT,	RO,	SE,	SI,	SK,	TR	
PRIORITY APPLN. INFO.:							1	KR 2	005-	833		1	A 20	0050	105			
											KR 2				_	A 20	0060	104
										Ī	WO 2	006-1	KR39		1	W 2	0060	105

OTHER SOURCE(S): MARPAT 145:146211

Provided are a photoreactive polymer that includes a multi-cyclic multicyclic compound at as its main chain and a method of preparing the same. The photoreactive polymer exhibits excellent thermal stability since it includes a multi-cyclic compound having a high glass transition temperature at as its main chain. In addition, the photoreactive polymer has a relatively large vacancy so that a photoreactive group can move relatively freely in the main chain therein. As a result, a slow photoreaction rate, which is a disadvantage of a conventional polymer material used to form an alignment layer for a liquid crystal display device, can be overcome.

872885-08-0

RL: CAT (Catalyst use); USES (Uses) (manufacture of photoreactive polymers)

RN 872885-08-0 ZCAPLUS

CN Borate(1-), tetrakis(pentafluorophenyl)-, hydrogen, compd. with tricyclohexylphosphine (1:1) (9CI) (CA INDEX NAME)

CM

CRN 118611-98-6 CMF C24 B F20 . H CCI CCS

$$F \qquad F \qquad F$$

$$F \qquad C \qquad F \qquad F$$

$$F \qquad F \qquad F$$

$$F \qquad F \qquad F$$

$$F \qquad F \qquad F$$

● H +

CM 2

CRN 2622-14-2 CMF C18 H33 P

REFERENCE COUNT:

THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L51 ANSWER 6 OF 24 ZCAPLUS COPYRIGHT 2007 ACS on STN ACCESSION NUMBER: 2006:31699 ZCAPLUS <u>Full-text</u>

4

DOCUMENT NUMBER:

144:108770

TITLE:

Method of producing cyclic olefin polymers having polar functional groups, olefin polymer produced using the method and optical anisotropic film comprising the

same

INVENTOR(S):

Yoon, Sung-Cheol; Won, Young-Chul; Park, Young-Whan; Chun, Sung-Ho; Choi, Dai-Seung; Kim, Won-Kook; Lim, Tae-Sun; Kim, Heon; Lee, Jung-Min; Paik, Kyung-Lim

PATENT ASSIGNEE(S):

LG Chem. Ltd., S. Korea PCT Int. Appl., 36 pp.

SOURCE:

CODEN: PIXXD2

DOCUMENT TYPE:

Patent English

LANGUAGE:

г: 2

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

CCI

CCS

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DATE
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                                                                    DATE
                                20060112
     WO 2006004376
                          A1
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             NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL,
             SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM,
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             CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH,
             GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
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     CN 1910210
                                20070207
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                                            CN 2005-80002113
                                                                    20050705
     EP 1765887
                          Α1
                                20070328
                                            EP 2005-765936
                                                                    20050705
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     JP 2007517958
                          Т
                                20070705
                                            JP 2006-549154
                                                                    20050705
     IN 2006DN03675
                          Α
                                20070803
                                            IN 2006-DN3675
                                                                    20060626
     KR 2007028488
                          Α
                                20070312
                                            KR 2007-7948
                                                                    20070125
PRIORITY APPLN. INFO.:
                                            KR 2004-52612
                                                                A 20040707
                                            KR 2004-74307
                                                               A 20040916
                                            WO 2005-KR2149
                                                                W 20050705
                                            WO 2005-KR2194
                                                                W 20050705
                                            KR 2005-61152
                                                                A3 20050707
OTHER SOURCE(S):
                         MARPAT 144:108770
     A method of producing a cyclic olefin polymer having a polar functional group
     and a high mol. weight with a high yield in which a catalyst is not
     deactivated due to polar functional groups, moisture and oxygen is provided.
     According to the olefin polymerization method, deactivation of a catalyst due
     to polar functional groups of monomers can be prevented, and thus a polyolefin
     having a high mol. weight can be prepared with a high yield, and the ratio of
     catalyst to monomer can be less than 1/5000 due to good activity of the
     catalyst, and thus removal of catalyst residues is not required.
IT
     872885-08-0P, Tricyclohexylphosphonium
     tetrakis(pentafluorophenyl)borate 872885-10-4P,
     Tri-tert-butylphosphonium tetrakis(pentafluorophenyl)borate
     RL: CAT (Catalyst use); IMF (Industrial manufacture); PREP (Preparation);
     USES (Uses)
        (method of producing cyclic olefin polymers having polar functional
       groups, olefin polymer produced using the method and optical
        anisotropic film comprising the same)
RN
     872885-08-0 ZCAPLUS
CN
     Borate(1-), tetrakis(pentafluorophenyl)-, hydrogen, compd. with
     tricyclohexylphosphine (1:1) (9CI) (CA INDEX NAME)
     CM
          1
         118611-98-6
    CRN
          C24 B F20 . H
     CMF
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$$F \qquad F \qquad F$$

$$F \qquad C \qquad F \qquad F$$

$$F \qquad F \qquad F$$

$$F \qquad F \qquad F$$

$$F \qquad F \qquad F$$

● H +

CM 2

CRN 2622-14-2 CMF C18 H33 P

RN 872885-10-4 ZCAPLUS

CN Borate(1-), tetrakis(pentafluorophenyl)-, hydrogen, compd. with tris(1,1-dimethylethyl)phosphine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 118611-98-6

CMF C24 B F20 . H

CCI CCS

$$F \qquad F \qquad F$$

$$F \qquad C \qquad F \qquad F$$

$$F \qquad C \qquad B \qquad A + - C \qquad F$$

$$F \qquad F \qquad F \qquad F$$

$$F \qquad F \qquad F \qquad F$$

● H +

CM 2

CRN 13716-12-6 CMF C12 H27 P

t-Bu t-Bu—P—Bu-t

REFERENCE COUNT:

THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L51 ANSWER 7 OF 24 ZCAPLUS COPYRIGHT 2007 ACS on STN

7

ACCESSION NUMBER:

2006:231929 ZCAPLUS Full-text

DOCUMENT NUMBER:

144:293248

TITLE:

Catalyst system for polymerizing cyclic olefin having polar functional group, polymerizing method using the catalyst system, olefin polymer produced by the method and optical anisotropic film comprising the olefin

polymer

INVENTOR(S):

Yoon, Sung Cheol; Won, Young Chul; Park, Young Whan; Chun, Sung Ho; Choi, Dai Seung; Kim, Won Kook; Lim, Taesun; Kim, Heon; Lee, Jung Min; Paik, Kyung Lim

PATENT ASSIGNEE(S):

: S. Korea

SOURCE:

U.S. Pat. Appl. Publ., 20 pp.

CODEN: USXXCO

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE		
US 2006058477	 A1	20060316	HE 2005 227002	20050016		
WO 2006031067	A1	20060316	US 2005-227093 WO 2005-KR3054	20050916		
WO 2006031067	A9	20061214	WO 2003-RR3034	20050915		
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CCI

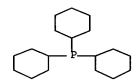
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             NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK,
             SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA,
             ZM, ZW
         RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
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             CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH,
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             KG, KZ, MD, RU, TJ, TM
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                                            EP 2005-808795
                                                                    20050915
             AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
             IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR
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                          Α
                                20070822
                                           CN 2005-80031322
                                                                    20050915
     KR 2007028488
                          Α
                                20070312
                                            KR 2007-7948
                                                                    20070125
     IN 2007DN02037
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                                20070817
                                            IN .2007-DN2037
                                                                   20070315
PRIORITY APPLN. INFO.:
                                            KR 2004-74307
                                                                A 20040916
                                            KR 2005-61152
                                                                Α
                                                                   20050707
                                            KR 2004-52612
                                                                Α
                                                                   20040707
                                            WO 2005-KR3054
                                                                   20050915
OTHER SOURCE(S):
                         MARPAT 144:293248
     A catalyst system capable of producing a cyclic olefin polymer having a polar
     functional group and a high mol. weight with a high yield in which a catalyst
     is not deactivated due to polar functional groups of monomers, and a method of
     producing polymers using the same are provided. The catalyst system for
     polymerization of olefin according to the invention has good thermal and
     chemical stability, and thus, in the method of preparing polyolefin using the
     catalyst system, the deactivation of a catalyst due to a polar functional
     group of the monomer is prevented, and thus a high yield of the cyclic olefin
     polymer with a high mol. weight can be obtained when a ratio of the catalyst
     to the monomer is 1:5000, and the removal of a catalyst residue is not
     required. The catalyst system is based on a complex of Ni, Pd, or Pt, a
     hydrocarbon group containing S, O, and N atoms bonded to the metal, and,
     optionally, another hydrocarbon group and a cocatalyst based on phosphonium
     compds. optionally having organic groups with O, S, Si, or N bonded to the P.
     Thus, 2-(3-acetyloxypropyl)-5-norbornene was polymerized in the presence of
     Pd(OAc)2 and tricyclohexylphosphonium tetrakis(pentafluorophenyl)borate in
     CH2Cl2 18 h at 90° to give polymer with weight-average mol. weight 250,071.
IT
     872885-08-0P, Tricyclohexylphosphonium
     tetrakis(pentafluorophenyl)borate 872885-10-4P,
     Tri-tert-butylphosphonium tetrakis(pentafluorophenyl)borate
     RL: CAT (Catalyst use); IMF (Industrial manufacture); PREP (Preparation);
     USES (Uses)
        (catalysts containing palladium, nickel, or platinum compds. and
        phosphonium compds. polymerizing cyclic olefins having polar functional
        groups for optical anisotropic films)
RN
     872885-08-0 ZCAPLUS
CN
     Borate(1-), tetrakis(pentafluorophenyl)-, hydrogen, compd. with
     tricyclohexylphosphine (1:1) (9CI) (CA INDEX NAME)
          1
     CM
     CRN
         118611-98-6
     CMF
         C24 B F20 . H
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H+

CM 2

CRN 2622-14-2 CMF C18 H33 P



872885-10-4 ZCAPLUS

RN Borate(1-), tetrakis(pentafluorophenyl)-, hydrogen, compd. with tris(1,1-dimethylethyl)phosphine (1:1) (9CI) (CA INDEX NAME) CN

CM 1

CRN 118611-98-6 CMF C24 B F20 . H

CCI CCS

$$F \qquad F \qquad F$$

$$F \qquad G \qquad F \qquad F$$

$$F \qquad F \qquad F$$

$$F \qquad F \qquad F$$

$$F \qquad F \qquad F$$

● H +

CM 2

CRN 13716-12-6 CMF C12 H27 P

t-Bu t-Bu—P—Bu-t

L51 ANSWER 8 OF 24 ZCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

2005:997731 ZCAPLUS Full-text

DOCUMENT NUMBER:

143:460249

TITLE:

Exploring the Influence of Ancillary Ligand Charge and

Geometry on the Properties of New Coordinatively

Unsaturated $Cp*(\kappa 2-P,N)Ru+$ Complexes: Linkage Isomerism, Double C-H Bond Activation, and Reversible

 α -Hydride Elimination

AUTHOR(S):

Rankin, Matthew A.; McDonald, Robert; Ferguson,

Michael J.; Stradiotto, Mark

CORPORATE SOURCE:

Department of Chemistry, Dalhousie University,

Halifax, NS, B3H 4J3, Can.

SOURCE:

Organometallics (2005), 24(21), 4981-4994

CODEN: ORGND7; ISSN: 0276-7333

PUBLISHER:

American Chemical Society

DOCUMENT TYPE:

Journal

LANGUAGE:

English

OTHER SOURCE(S):

CASREACT 143:460249

The synthesis, characterization, and reactivity properties of new Cp*Ru complexes supported by $\kappa2\text{-P}, N\text{-1-PiPr}2\text{-2-NMe}2\text{-indene}$ (1a), $\kappa2\text{-P}, N\text{-2-NMe}2\text{-3-PiPr}2\text{-indene}$ (1b), and $\kappa2\text{-P}, N\text{-2-NMe}2\text{-3-PiPr}2\text{-}$ indenide (1) are described (Cp* = $\eta5\text{-C5Me}5$). Addition of 1a to (Cp*RuCl)4 afforded Cp*Ru(Cl)($\kappa2\text{-P}, N\text{-1a}$) (2a, 92%), which in turn was transformed into Cp*Ru(Cl)($\kappa2\text{-P}, N\text{-1b}$) (2b, 85%). Treatment of either 2a or 2b with AgBF4 in MeCN provided the corresponding 18-electron, base-stabilized cation [Cp*Ru(MeCN)($\kappa2\text{-P}, N\text{-1a}, b$)]+BF4- (3a, 89%; 3b, 91%). In the pursuit of the analogous MeCN-free, 16-electron species (4a or

4b), complexes 2a or 2b were treated with Li(Et20)2.5B(C6F5)4. In the case of 2a, the linkage isomer $[Cp*Ru(\eta6-1a)]+B(C6F5)4-(endo-4c, 74%)$ was obtained; exposure of this complex to NEt3 afforded $[Cp*Ru(\eta6-1b)]+B(C6F5)4-(4d, 85%)$. In contrast, chloride abstraction from 2b generated the C-H bond activation product 4e (83%); variable-temperature NMR data revealed that the apparent cyclometalation of 4b to give 4e is reversible. While the base-stabilized zwitterion 5a MeCN was successfully prepared (83%), attempts to generate the coordinatively unsatd. zwitterion Cp*Ru(K2-P,N-1) (5a) instead gave the isomeric hydridocarbenes 5b (80%) and 5c (84%). The apparent rearrangement of 5a to a hydridocarbene is noteworthy, as it represents a remarkably facile, ligand-assisted double geminal C-H bond activation process. Also, data obtained from 1-dimensional- and 2-dimensional-EXSY NMR expts. involving 5c provided compelling evidence for what appears to be the 1st documented interconversion of Ru(H):CH and Ru-CH2 groups by way of reversible α -hydride elimination. In keeping with this dynamic process, treatment of 5c with PHPh2 afforded the alkylruthenium adduct 6 (70%). Single-crystal x-ray diffraction data are provided for 2a, 2b, 3a, 3b·1.5C5H12, 4d, 4e, (5a·MeCN)·0.5MeCN, 5c, and $6 \cdot 0.5 \text{C5H12}$.

IT 869006-09-7P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (crystal structure; preparation, structure, linkage isomerism, double C-H bond activation, and reversible α -hydride elimination of coordinatively unsatd. ruthenium P-N indenide metallacyclic complexes)

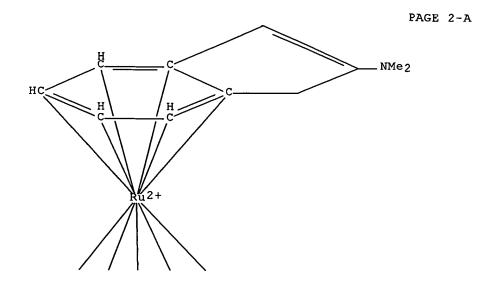
RN 869006-09-7 ZCAPLUS

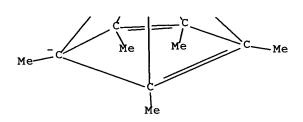
CN Ruthenium(1+), $[(3a,4,5,6,7,7a-\eta)-3-[bis(1-methylethyl)phosphino]-N,N-dimethyl-1H-inden-2-amine][(1,2,3,4,5-\eta)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]-, tetrakis(pentafluorophenyl)borate(1-) (9CI) (CA INDEX NAME)$

CM 1

CRN 869006-08-6 CMF C27 H41 N P Ru CCI CCS

PAGE 1-A





PAGE 3-A

CM 2

CRN 47855-94-7

CMF C24 B F20

CCI CCS

IT 869006-05-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation, structure, linkage isomerism, double C-H bond activation, and reversible α -hydride elimination of coordinatively unsatd.

ruthenium P-N indenide metallacyclic complexes)

RN 869006-05-3 ZCAPLUS

CN Ruthenium(1+), [(3a,4,5,6,7,7a-η)-1-[bis(1-methylethyl)phosphino]-N,N-dimethyl-1H-inden-2-amine][(1,2,3,4,5-η)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]-, stereoisomer, tetrakis(pentafluorophenyl)borate(1-)(9CI) (CA INDEX NAME)

CM 1

CRN 869006-04-2 CMF C27 H41 N P Ru CCI CCS

PAGE 1-A

HC
HC
P(Pr-i)2

PAGE 2-A

CM 2

CRN 47855-94-7 CMF C24 B F20 CCI CCS

REFERENCE COUNT: 87 THERE ARE 87 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L51 ANSWER 9 OF 24 ZCAPLUS COPYRIGHT 2007 ACS on STN ACCESSION NUMBER: 2005:283905 ZCAPLUS Full-text

DOCUMENT NUMBER:

143:18679

TITLE:

Dihydrogen Complexes of Rhodium: [RhH2(H2)x(PR3)2]+ (R

= Cy, iPr; x = 1, 2)

AUTHOR(S):

Ingleson, Michael J.; Brayshaw, Simon K.; Mahon, Mary

F.; Ruggiero, Giuseppe D.; Weller, Andrew S.

CORPORATE SOURCE:

Department of Chemistry, University of Bath, Bath, BA2

7AY, UK

SOURCE:

Inorganic Chemistry (2005), 44(9), 3162-3171

CODEN: INOCAJ; ISSN: 0020-1669

PUBLISHER:

American Chemical Society

DOCUMENT TYPE:

Journal

LANGUAGE:

English

OTHER SOURCE(S):

CASREACT 143:18679

AB Addition of H2 (4 atm at 298 K) to [Rh(nbd)(PR3)2][BArF4] [R = Cy, iPr] affords Rh(III) dihydride/dihydrogen complexes. For R = Cy, complex [Rh(H)2(η2-H2)2(PCy3)2][BArF4] (1a) results, which was characterized by low-

temperature NMR expts. An x-ray diffraction study on 1a confirmed the $\{Rh(PCy3)2\}$ core structure, but due to a poor data set, the H ligands were not located. DFT calcns. at the B3LYP/DZVP level support the formulation as a Rh(III) dihydride/dihydrogen complex with cis hydride ligands. For R = iPr, the equivalent species, $[Rh(H)2(\eta2-H2)2(PiPr3)2][BArF4]$ (2a), is formed, along with another complex that was spectroscopically identified as the monodihydrogen, bis-hydride solvent complex $[Rh(H)2(\eta2-H2)(PiPr3)2][BArF4]$ (2b). The analogous complex with PCy3 ligands, $[Rh(H)2(\eta2-H2)(CD2C12)(PCy3)2][BArF4]$ (1b), can be observed by reducing the H2

[Rh(H)2(n2-H2)(CD2Cl2)(PCy3)2][BArF4] (lb), can be observed by reducing the H2 pressure to 2 atm (at 298 K). Under vacuum, the dihydrogen ligands are lost in these complexes to form the spectroscopically characterized species, tentatively identified as the bis hydrides [Rh(H)2(L)2(PR3)2][BArF4] (lc, R = Cy; 2c, R = iPr; L = CD2Cl2 or agostic interaction). Exposure of lc or 2c to a H2 atmosphere regenerates the dihydrogen/bis-hydride complexes, while adding MeCN affords the bis-hydride MeCN adduct complexes

[Rh(H)2(NCMe)2(PR3)2][BArF4]. The dihydrogen complexes lose [HPR3][BArF4] at or just above ambient temperature, suggested to be by heterolytic splitting of coordinated H2, to ultimately afford the dicationic cluster compds.

[Rh6(PR3)6(μ -H)12][BArF4]2 in moderate yield.

IT 852244-08-7 852244-09-8

RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)

(acid dissociation constant and formation in heterolytic splitting of dihydrogen in rhodium dihydrogen hydride phosphine complexes)

RN 852244-08-7 ZCAPLUS

Borate(1-), tetrakis[3,5-bis(trifluoromethyl)phenyl]-, hydrogen, compd. with tricyclohexylphosphine (1:1) (9CI) (CA INDEX NAME)

CM 1

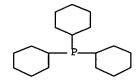
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CRN 121281-53-6 CMF C32 H12 B F24 . H CCI CCS

● H+

CM 2

CRN 2622-14-2 CMF C18 H33 P



RN 852244-09-8 ZCAPLUS

Borate(1-), tetrakis[3,5-bis(trifluoromethyl)phenyl]-, hydrogen, compd. CN with tris(1-methylethyl)phosphine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 121281-53-6

C32 H12 B F24 . H CMF

CCI CCS

CM 2

CRN 6476-36-4 CMF C9 H21 P

i-Pr i-Pr-P-Pr-i

REFERENCE COUNT:

55 THERE ARE 55 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L51 ANSWER 10 OF 24 ZCAPLUS COPYRIGHT 2007 ACS on STN ACCESSION NUMBER: 2003:952941 ZCAPLUS Full-text

DOCUMENT NUMBER:

140:146275

TITLE:

Coordinating Anions: (Phosphino)tetraphenylborate

Ligands as New Reagents for Synthesis Thomas, Christine M.; Peters, Jonas C.

AUTHOR(S): CORPORATE SOURCE:

Division of Chemistry and Chemical Engineering, Arnold

and Mabel Beckman Laboratories of Chemical Synthesis, California Institute of Technology, Pasadena, CA.

91125, USA

SOURCE:

Inorganic Chemistry (2004), 43(1), 8-10

CODEN: INOCAJ; ISSN: 0020-1669

PUBLISHER:

American Chemical Society

DOCUMENT TYPE: LANGUAGE: Journal English

OTHER SOURCE(S):

CASREACT 140:146275

Anionic, electron-releasing phosphines that incorporate a borate counter-anion within the ligand framework are promising reagents for organometallic catalysis. This report describes the synthesis of a new class of monodentate tertiary phosphines built upon the commonly employed tetraphenylborate anion. These new phosphines are highly stable and strongly electron-releasing and readily coordinate transition metals. Moreover, they are promising reagents for catalysis, as demonstrated by their ability to promote the Suzuki cross-coupling of aryl chloride substrates. Thus, lithiation of m-BrC6H4PiPr2 (preparation given) with t-BuLi in THF/pentane followed by sequential treatment with Ph3B and Bu4NBr gave 48% title ligand, [Bu4N][Ph3BPm-iPr2] (crystal structure), which cocatalyzes Suzuki cross-coupling reaction of PhB(OH)2 with 1,4-dichlorobenzene in the presence of Pd2(dba)3 to give 4-chlorobiphenyl.

IT 651329-77-0P

RL: CAT (Catalyst use); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent); USES (Uses) (crystal structure; preparation of (phosphino)tetraphenylborate coordinating

anion ligands as cocatalysts for transition metal catalyzed Suzuki cross-coupling reaction of arylboronic acid with aryl halide)

RN 651329-77-0 ZCAPLUS

CN 1-Butanaminium, N,N,N-tributyl-, (T-4)-[3-[bis(1-methylethyl)phosphino]phenyl]triphenylborate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 651329-76-9 CMF C30 H33 B P CCI CCS

CM 2

CRN 10549-76-5 CMF C16 H36 N

IT 651330-05-1P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (crystal structure; preparation of (phosphino)tetraphenylborate coordinating

anion ligands as cocatalysts for transition metal catalyzed Suzuki cross-coupling reaction of arylboronic acid with aryl halide)

RN 651330-05-1 ZCAPLUS

CN Ethanaminium, N,N,N-triethyl-, (T-4)-[3-[bis(1-methylethyl)phosphino]phenyl]triphenylborate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 651329-76-9 CMF C30 H33 B P CCI CCS

CM 2

CRN 66-40-0 CMF C8 H20 N

IT 651329-79-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of (phosphino)tetraphenylborate coordinating anion ligands as cocatalysts for transition metal catalyzed Suzuki cross-coupling reaction of arylboronic acid with aryl halide)

RN 651329-79-2 ZCAPLUS

CN 1-Butanaminium, N,N,N-tributyl-, (T-4)-[4-[bis(1-methylethyl)phosphino]phenyl]triphenylborate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 651329-78-1 CMF C30 H33 B P

CCI CCS

CM 2

CRN 10549-76-5 CMF C16 H36 N

REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L51 ANSWER 11 OF 24 ZCAPLUS COPYRIGHT 2007 ACS on STN ACCESSION NUMBER: 2001:886259 ZCAPLUS Full-text

DOCUMENT NUMBER:

136:20365

TITLE:

Preparation of transition metal complexes as catalyst

for polymerization of olefins

INVENTOR(S): Johnson, Lynda K.; Bennett, Alison M. A.; Dobbs,

Kerwin D.; Ionkin, Alex S.; Ittel, Steven D.; Wang,

Ying; Radzewich, Catherine E.; Wang, Lin

PATENT ASSIGNEE(S):

E. I. Du Pont de Nemours & Co., USA

SOURCE:

PCT Int. Appl., 79 pp.

DOCUMENT TYPE:

CODEN: PIXXD2

DOCOMENT TIPE.

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001092347	A 2	20011206	WO 2001-US17628	20010531

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WO 2001092347
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             LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO,
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             VN, YU, ZA, ZW
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PRIORITY APPLN. INFO.:
                                             US 2000-208087P
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                                             US 2002-57090
                                                                  A3 20020125
OTHER SOURCE(S):
                         MARPAT 136:20365
     Polymers are produced using transition metal complexes that have sites capable
     of binding a Lewis acid in close proximity to the metal center. The patent
     also relates to a process for polymerizing an olefin component comprising one
     or more polymerizable olefins, comprising the step of contacting, under
     polymerizing conditions, said olefin component with a polymerization catalyst
     system, characterized in that the polymerization catalyst system comprises a
     group 3-11 transition metal or lanthanide, a coordinating ligand, and a Lewis
     acid component, wherein the Lewis acid component is : (a) neutral and
     covalently bound to said coordinating ligand, or (b) pos. charged and bound to
     a Lewis basic site of said coordinating ligand. The transition metal is Fe,
     CO, Pd, Ni or Cu.
ΙT
     378793−55−6₽
     RL: CAT (Catalyst use); IMF (Industrial manufacture); PREP (Preparation);
        (preparation of transition metal complexes as catalyst for polymerization
of
        olefins)
RN
     378793-55-6 ZCAPLUS
     Nickel(1+), [1-[bis(1,1-dimethylethyl)phosphino-\kappa P]-3-[bis(1,1-dimethylethyl)phosphino-\kappa P]
CN
     dimethylethyl)phosphino]-1,3-dihydro-2H-inden-2-one-κΟ][(1,2,3-
     η)-2-(methoxycarbonyl)-2-propenyl]-, tetrakis(pentafluorophenyl)borate
```

CM 1

(1-) (9CI) (CA INDEX NAME)

CRN 378793-54-5

CMF C30 H49 Ni O3 P2

CCI CCS

PAGE 1-A

$$t-Bu$$
 $t-Bu$
 $t-Bu$

PAGE 2-A

IJ

CM 2

CRN 47855-94-7

CMF C24 B F20

cci ccs

L51 ANSWER 12 OF 24 ZCAPLUS COPYRIGHT 2007 ACS on STN ACCESSION NUMBER: 1991:583554 ZCAPLUS Full-text

DOCUMENT NUMBER:

115:183554

TITLE:

Rhodium(I) and iridium(I) complexes with

1,2-bis(dicyclohexylphosphino)ethane ligands, and

their reactions with carbon monoxide

AUTHOR(S):

Del Zotto, Alessandro; Costella, Luigina; Mezzetti,

Antonio; Rigo, Pierluigi

CORPORATE SOURCE:

Ist. Chim., Univ. Udine, Udine, 33100, Italy

SOURCE:

Journal of Organometallic Chemistry (1991), 414(1),

109-18

CODEN: JORCAI; ISSN: 0022-328X

DOCUMENT TYPE:

Journal

LANGUAGE: English

1,2-Bis(dicyclohexylphosphino)ethane (dcpe) forms the mononuclear, squareplanar rhodium(I) and iridium(I) complexes [M(COD)(dcpe)]BPh4 (COD = 1,5cyclooctadiene), [M(dcpe)2]BPh4, and [MCl(CO)(dcpe)], which have been characterized by elemental analyses, IR, and 1H and 31P{1H} NMR spectroscopy. Their behavior toward carbon monoxide in dichloromethane solution at different temps. was examined, and the nature of the products formed established by IR and 31P{1H} NMR spectroscopy. Some of the products, including [M(CO)2(dcpe)]BPh4 and [Ir(COD)(CO)(dcpe)]BPh4, were isolated in the solid state and fully characterized. The catalytic activity of the rhodium derivs. in the decarbonylation of benzaldehyde has been studied, and compared with that of the analogous complexes containing phenyl-substituted diphosphines.

IT 136638-35-2P

> RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

136638-35-2 ZCAPLUS RN

Iridium(1+), dicarbonyl[1,2-ethanediylbis[dicyclohexylphosphine]-P][1,2-CN ethanediylbis[dicyclohexylphosphine]-P,P']-, (TB-5-12)-, tetraphenylborate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 136638-34-1

CMF C54 H96 Ir O2 P4

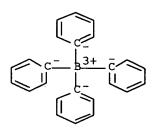
CCI CCS

PAGE 1-A

PAGE 2-A

CM

CRN 4358-26-3 CMF C24 H20 B CCI CCS



L51 ANSWER 13 OF 24 ZCAPLUS COPYRIGHT 2007 ACS on STN ACCESSION NUMBER: 1982:162905 ZCAPLUS Full-text

DOCUMENT NUMBER:

96:162905

AUTHOR(S):

TITLE:

Iron(II), cobalt(II) and nickel(II) complexes with the tripod ligand tris(2-dicyclohexylphosphinoethyl)amine

Stoppioni, P.; Morassi, R.; Zanobini, F.

CORPORATE SOURCE: Ist. Chim. Gen. Inorg., Univ. Florence, Florence,

Inorganica Chimica Acta (1981), 52(1), 101-6 SOURCE:

CODEN: ICHAA3; ISSN: 0020-1693

DOCUMENT TYPE:

Journal

LANGUAGE: English

The title tripod ligand (Cynp3), sterically hindered at the three P atoms, forms complexes [MX(Cynp3)]Y, (M = Co, Ni, X = Cl, Br, I, NCS, Y = BPh4; M =Fe, X = Cl, Br, I, Y = BPh4; M = Co, X = Y = Cl, Br, I, NCS; M = Fe, X = Y =NCS). The Fe complexes are five-coordinate with a trigonal bipyramidal structure. The Ni complexes are four-coordinate (donor set NP2X) with a square planar geometry and a non-bonded phosphine group. The Co complexes [CoX(Cynp3)]BPh4 are high-spin five-coordinate with a distorted trigonal bipyramidal geometry both in the solid state and in solution In the [CoX(Cynp3)]X complexes the ligand is tetradentate in the solid state, whereas in solution tetrahedral species containing bidentate attachments (donor set P2X2) are also formed. Two isomeric bis-thiocyanate derivs. have been obtained, one blue and one brown. The former is high-spin with a pseudotetrahedral geometry, whereas the latter is low-spin with a trigonal bipyramidal geometry and donor set NP2(NCS)2. In solution, both complexes give the same trigonal bipyramidal species.

81433-15-0P 81433-17-2P 81433-19-4P IT 81433-21-8P

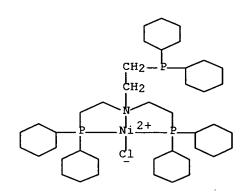
> RL: SPN (Synthetic preparation); PREP (Preparation) (preparation and spectral characteristics of)

RN 81433-15-0 ZCAPLUS

Nickel(1+), chloro[2-(dicyclohexylphosphino)-N,N-bis[2-CN (dicyclohexylphosphino)ethyl]ethanamine-N,P,P']-, (SP-4-3)-, tetraphenylborate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 81433-14-9 CMF C42 H78 Cl N Ni P3 CCI CCS.



CM 2

CRN 4358-26-3 CMF C24 H20 B CCI CCS

RN 81433-17-2 ZCAPLUS

CN Nickel(1+), bromo[2-(dicyclohexylphosphino)-N,N-bis[2-(dicyclohexylphosphino)ethyl]ethanamine-N,P,P']-, (SP-4-3)-, tetraphenylborate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 81433-16-1 CMF C42 H78 Br N Ni P3

CCI CCS

CM 2

CRN 4358-26-3 CMF C24 H20 B CCI CCS

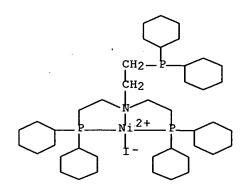
RN 81433-19-4 ZCAPLUS
CN Nickel(1+), [2-(dicyclohexylphosphino)-N,N-bis[2-(dicyclohexylphosphino)ethyl]ethanamine-N,P,P']iodo-, (SP-4-3)-, tetraphenylborate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 81433-18-3

CMF C42 H78 I N Ni P3

CCI CCS



CM 2

CRN 4358-26-3 CMF C24 H20 B CCI CCS

RN 81433-21-8 ZCAPLUS
CN Nickel(1+), [2-(dicyclohexylphosphino)-N,N-bis[2-(dicyclohexylphosphino)ethyl]ethanamine-N,P,P'](thiocyanato-N)-, (SP-4-1)-, tetraphenylborate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 81433-20-7

CMF C43 H78 N2 Ni P3 S

CCI CCS

CM 2

CRN 4358-26-3 CMF C24 H20 B

CCI CCS

L51 ANSWER 14 OF 24 ZCAPLUS COPYRIGHT 2007 ACS on STN ACCESSION NUMBER: 1973:72347 ZCAPLUS Full-text

DOCUMENT NUMBER: 78:72347

ORIGINAL REFERENCE NO.: 78:11509a,11512a

TITLE:

Transition metal-carbon bonds. XXXIII. Internal metalations of secondary and tertiary carbon atoms by

platinum(II) and palladium(II)

AUTHOR(S):

Gill, D. F.; Mann, B. E.; Shaw, B. L.

CORPORATE SOURCE:

Sch. Chem., Univ. Leeds, Leeds, UK

SOURCE:

Journal of the Chemical Society, Dalton Transactions: Inorganic Chemistry (1972-1999) (1973), (3), 270-8

CODEN: JCDTBI; ISSN: 0300-9246

DOCUMENT TYPE:

Journal English

LANGUAGE:

Treating [PtCl2(PhCN)2] with di-tert-butyl(o-ethylphenyl)phosphine (HL) or ditert-butyl(o-isopropylphenyl)phosphines (HL1) gave the internally metalated complexes [Pt2Cl2(P-C)2] (P-C = CHMeC6H4P(CMe3)2 or P1-C = CMe2C6H4P(CMe3)2, resp.). Treating Na2PdCl4 with HL gave trans-[PdCl2L2] which on heating gave PdCl2(P-C)2]. In all cases the metalation occurred at the α -C of the ligand.

[M2Cl2(P-C)2] (M = Pt, Pd) undergo bridge-splitting reactions with various ligands Q (e.g. py, PPh3, PMe2Ph) to give mononuclear species [MClQ(P-C)]. Treatment of Na2PdCl4 with HL1 gave [Pd2Cl4L21] which did not internally metalate. 1H, 13C, and 31P NMR spectra were measured and discussed.

IT 40988-98-5P 41574-12-3P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and complexation with palladium and platinum salts)

RN 40988-98-5 ZCAPLUS

CN Borate(1-), tetraphenyl-, hydrogen, compd. with bis(1,1-dimethylethyl)[2-(1-methylethyl)phenyl]phosphine(1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 35823-26-8 CMF C17 H29 P

CM 2

CRN 33906-65-9 CMF C24 H20 B . H CCI CCS

● H+

RN 41574-12-3 ZCAPLUS

CN Borate(1-), tetraphenyl-, hydrogen, compd. with bis(1,1-dimethylethyl)(2-ethylphenyl)phosphine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 35823-27-9 CMF C16 H27 P

CM 2

CRN 33906-65-9 CMF C24 H20 B . H

CCI CCS

● H⁺

IT 40988-98-5P 41574-12-3P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 40988-98-5 ZCAPLUS

CN Borate(1-), tetraphenyl-, hydrogen, compd. with bis(1,1-dimethylethyl)[2-(1-methylethyl)phenyl]phosphine(1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 35823-26-8 CMF C17 H29 P

CM 2

CRN 33906-65-9 CMF C24 H20 B . H

CCI CCS

● н+

RN 41574-12-3 ZCAPLUS

CN Borate(1-), tetraphenyl-, hydrogen, compd. with bis(1,1-dimethylethyl)(2-ethylphenyl)phosphine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 35823-27-9 CMF C16 H27 P

CM 2

CRN 33906-65-9 CMF C24 H20 B . H CCI CCS

● #+

L51 ANSWER 15 OF 24 ZCAPLUS COPYRIGHT 2007 ACS on STN ACCESSION NUMBER: 1968:418348 ZCAPLUS <u>Full-text</u>

DOCUMENT NUMBER:

69:18348

ORIGINAL REFERENCE NO.:

69:3423a,3426a

TITLE:

Chemistry of alkylenephosphines. IV. Kinetic studies

of triphenylalkylenephosphine hydrolysis

AUTHOR(S):

Issleib, Kurt; Lindner, Rolf

CORPORATE SOURCE:

Univ. Halle/Saale, Halle/Saale, Fed. Rep. Ger.

SOURCE:

Justus Liebigs Annalen der Chemie (1968), 713, 12-29

CODEN: JLACBF; ISSN: 0075-4617

DOCUMENT TYPE:

Journal German

LANGUAGE:

In aqueous solution Ph3P:CHPPh3Br forms Ph3PO, C6H6 and Ph2MePO via Ph3PMeBr. AΒ The kinetics of the hydrolysis are studied by uv spectrophotometric measurement of the ylene concentration relative to temperature and pH. constant pH the reaction rate of the alkylene phosphine cleavage is of first order. Assuming that [H3O+] << Kal, pH-dependent hydrolysis was not detected. When pH <<pKal the decomposition rate of the ylene is decreased by an acidbase equilibrium The temperature-dependence of the rate consts. led to the activation enthalpy $\Delta H++=7.4$ kcal./mole and activation entropy $\Delta S++=-61$ cal. mole-1. The reaction mechanism of the hydrolysis is discussed. The hydrolysis of Ph3P:CRPR21Ha1 (I) and Ph3P:CHCOR was also studied. The preparation of I from Ph3P:CRPR21 and alkyl halides is described. 45 references.

IT 15389-64-7P 20346-90-1P

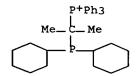
> RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

15389-64-7 ZCAPLUS RN

CN Phosphonium, [1-(dicyclohexylphosphino)-1-methylethyl]triphenyl-, tetraphenylborate(1-) (8CI) (CA INDEX NAME)

CM 1

CRN 47757-17-5 CMF C33 H43 P2



2 CM

CRN 4358-26-3 CMF C24 H20 B CCI CCS

RN 20346-90-1 ZCAPLUS

CN Phosphonium, [1-(diethylphosphino)-1-methylethyl]triphenyl-, tetraphenylborate(1-) (8CI) (CA INDEX NAME)

CM 1

CRN 47519-93-7 CMF C25 H31 P2

PEt 2 Me-C-Me P+Ph3

CM 2

CRN 4358-26-3 CMF C24 H20 B CCI CCS

C - 3+ C

L51 ANSWER 16 OF 24 ZCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

1967:46454 ZCAPLUS <u>Full-text</u>

DOCUMENT NUMBER:

66:46454

ORIGINAL REFERENCE NO.:

66:8823a,8826a

TITLE:

Chemistry of phosphine alkylenes. I. Reaction of

phosphine alkylenes with dialkyl and diaryl

chlorophosphines

AUTHOR(S):

Issleib, Kurt; Lindner, Rolf

CORPORATE SOURCE:

Univ. Halle, Halle, Germany

SOURCE:

Ann. Chem., Justus Liebigs

CODEN: ACJLAO

(1966), 699, 40-52

DOCUMENT TYPE:

Journal

LANGUAGE:

German

Substituted triphenyl- and tricyclohexylphosphine alkylenes [RR1C:PPh3 (I) and RR1C:P(C6H11)3] react with R22PCl [R2 = Ph and R2 = C6H11] with nucleophilic substitution to give (R22PCRRP+PH3)X-, R22PCR:PPh3, and R22PCR:P(C6H11)3 (II) where C6H11 is cyclohexyl. II were characterized by reaction with H2O and alkyl halides and give with BzH (a Wittig reaction), the tertiary phosphines PhCH:CMeOR22. Ph3P was isolated as a by-product of these reactions in varying amts. depending on the substituents. The mechanism of the reaction was discussed. Solns. of appropriate I were prepared from the corresponding phosphonium salts by the NaNH2 method (Bestmann, CA 56, 12925b).

IT 15389-63-6P 15389-64-7P

RN 15389-63-6 ZCAPLUS

CN Phosphonium, [α -(diethylphosphino)- α -methylphenethyl]triphenyl, tetraphenylborate(1-) (8CI) (CA INDEX NAME)

CM 1

CRN 47717-29-3 CMF C31 H35 P2

CM 2

CRN 4358-26-3 CMF C24 H20 B CCI CCS

RN 15389-64-7 ZCAPLUS

CN Phosphonium, [1-(dicyclohexylphosphino)-1-methylethyl]triphenyl-, tetraphenylborate(1-) (8CI) (CA INDEX NAME)

CM 1

CRN 47757-17-5 CMF C33 H43 P2

CM 2

CRN 4358-26-3 CMF C24 H20 B CCI CCS

L51 ANSWER 17 OF 24 BABS COPYRIGHT 2007 BEILSTEIN MDL on STN DUPLICATE 3

ACCESSION NUMBER:

TITLE:

6281441 BABS <u>Full-text</u>

An Acidity Scale for Phosphorus-Containing Compounds Including Metal Hydrides and Dihydrogen Complexes in

THF: Toward the Unification of Acidity Scales

AUTHOR(S): Abdur-Rashid, Kamaluddin; Fong, Tina P.; Greaves,

Bronwyn; Gusev, Dmitry G.; Hinman, Justin G.; Landau,

Shaun E.; Lough, Alan J.; Morris, Robert H. J.Amer.Chem.Soc. (2000), 122(38), 9155 - 9171

CODEN: JACSAT

DOCUMENT TYPE:

LANGUAGE:

SOURCE:

Journal English

SUMMARY LANGUAGE:

English

ABSTRACT:

More than 70 equilibrium constants K between acids and bases, mainly phosphine derivatives,

have been

measured in tetrahydrofuran (THF) at

20 deg C by 1H

and/or 31P NMR. The acids were

chosen or newly

synthesized in order to cover the wide pK&\$a%%THF& range of 5-41 versus the anchor compound [HPCy3]BPh4 at 9.7. These pK&\$a%*THF& values are approximations to absolute, free ion pK&a%%THF& and are obtained by crudely correcting the observed K for 1:1 ion-pairing effects by use of the Fuoss equation. The acid/base compounds include 14 phosphonium/phosphine couples, 17 cationic hydride/neutral hydride couples, 9 neutral polyhydride/anionic hydride couples, 14 dihydrogen/hydride couples, and 4 other nitrogen- and phosphorus-based acids. The effects on pK&a% of the counterions BAr'4%-& and BF4%-& and [K(2,2,2-crypt)]%+& versus [K(18crown-6)]%+& are found to be minor after correcting for differences in inter-ion distances in the ion-pairs involved. Correlations with \$n(M-H) noted here for the first time suggest that destabilization of M-H bonding in the conjugate base hydride is an important contributor to hydride acidity. It appears that Re-H bonding in the anions [ReH6(PR3)2]%-& is greatly weakened by small increases in the basicity of PR3, resulting in a large increase in the pK&\$a% of the conjugate acid ReH7(PR3)2. Correlations with other scales allow an estimate of the pK&\$a%%THF& values of more than 1000 inorganic and organic acids, 20 carbonyl hydride complexes, 46 cationic hydrides complexes, and dihydrogen gas. Therefore, many new acid-base reactions can be predicted and known reactions explained. THF, with its low dielectric constant, disfavors the ionization of neutral acids HA over

HB%+&, and therefore separate lines

are found for

pK&\$a%%THF&(HA) and

pK&\$a%%THF&(HB#+&) when plotted

against pK&a##DMSO& or pK&a##MeCN&.

The crystal

structure of [Re(H)2(PMe3)5]BPh4 is

reported.

L51 ANSWER 18 OF 24 BEILSTEIN COPYRIGHT 2007 BEILSTEIN MDL on STN

Beilstein Records (BRN):
Lin. Struct. Formula (LSF):
Fragm. Molec. Formula (FMF):
Molecular Formula (MF):
Molecular Weight (MW):
Fragment BRN (FBRN):
Lawson Number (LN):
Compound Type (CTYPE):
Constitution ID (CONSID):

8819356 C24H20B(1-)*C12H27P*H(1+) C24 H20 B , C12 H27 P , H C24 H20 B . C12 H27 P . H 319.23, 202.32, 1.01 1654829, 1738613, 3902898 16763, 3758

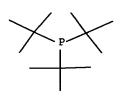
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Constitution ID (CONSID): 7465252
Tautomer ID (TAUTID): 8287899
Entry Date (DED): 2001/07/25
Update Date (DUPD): 2007/02/05

CM 1

FBRN 3902898 FMF H

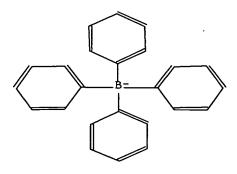
CM 2

FBRN 1738613 FMF C12 H27 P



CM 3

FBRN 1654829 FMF C24 H20 B



Field Availability:

Code	Name	Occurrence
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BRN	Beilstein Records	1
LSF	Linearized Structure Formula	1
FMF	Fragment Molecular Formula	3
MF	Molecular Formula	1
FW	Formular Weight	3
FBRN	Fragment BRN	3
LN	Lawson Number	2
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
DED	· Entry Date	1
DUPD	Update Date	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
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RX	Reaction Documents	2
RXREA	Substance is Reaction Reactant	1
RXPRO	Substance is Reaction Product	1

All References:

ALLREF

- Abdur-Rashid, Kamaluddin; Fong, Tina P.; Greaves, Bronwyn; Gusev, Dmitry G.; Hinman, Justin G.; Landau, Shaun E.; Lough, Alan J.; Morris, Robert H., J. Am. Chem. Soc., CODEN: JACSAT, SIN122(38), <2000>, 9155 - 9171; BABS-6594776
- Abdur-Rashid, Kamaluddin; Fong, Tina P.; Greaves, Bronwyn; Gusev, Dmitry G.; Hinman, Justin G.; Landau, Shaun E.; Lough, Alan J.; Morris, Robert H., J.Amer.Chem.Soc., CODEN: JACSAT, 122(38), <2000>, 9155 - 9171; BABS-6281441

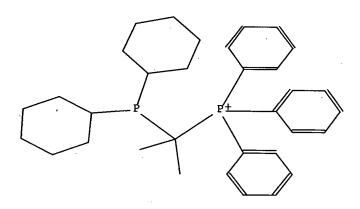
L51 ANSWER 19 OF 24 BEILSTEIN COPYRIGHT 2007 BEILSTEIN MDL on STN

Beilstein Records (BRN):
Lin. Struct. Formula (LSF):
Fragm. Molec. Formula (FMF):
Molecular Formula (MF):
Molecular Weight (MW):
Fragment BRN (FBRN):
Lawson Number (LN):
Compound Type (CTYPE):
Beilstein Citation (BSO):
Entry Date (DED):
Update Date (DUPD):
Compound Disposition (CDISP):

6710863 C33H43P2(1+)*C24H20B(1-) C33 H43 P2 , C24 H20 B C33 H43 P2 . C24 H20 B 501.65, 319.23 4163294, 3910925 16763, 16731, 16723, 709 isocyclic 5-16 1994/07/15 1994/07/22 4115452 Alternate BRN

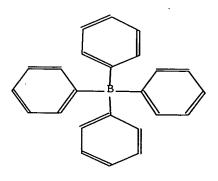
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FBRN 4163294 FMF C33 H43 P2



CM 2

FBRN 3910925 FMF C24 H20 B



Fragment Notes:

Unknown location for Localized Charge of (-1)

Field Availability:

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LN	Lawson Number	4 ⁻
FS	File Segment	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
DED	Entry Date	. 1
DUPD	Update Date	1
CDISP	Compound Disposition	1
MP	Melting Point	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
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RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

All References:

ALLREF

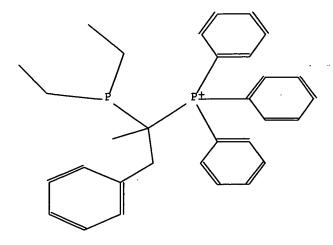
1. Issleib, K.; Lindner, R., Justus Liebigs Ann. Chem., CODEN: JLACBF, 699, <1966>, 40-52

L51 ANSWER 20 OF 24 BEILSTEIN COPYRIGHT 2007 BEILSTEIN MDL on STN

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                                6710850
Lin. Struct. Formula (LSF):
                                C31H35P2(1+)*C24H20B(1-)
Fragm. Molec. Formula (FMF):
                                C31 H35 P2 , C24 H20 B
Molecular Formula (MF):
                                C31 H35 P2 . C24 H20 B
Molecular Weight (MW):
                                469.57, 319.23
Fragment BRN (FBRN):
                                4160575, 3910925
Lawson Number (LN):
                                16763, 16731, 7144, 3746
Compound Type (CTYPE):
                                isocyclic
Beilstein Citation (BSO):
                                5-16
Entry Date (DED):
                               1994/07/15
Update Date (DUPD):
                               1994/07/22
Compound Disposition (CDISP): 4115096 Alternate BRN
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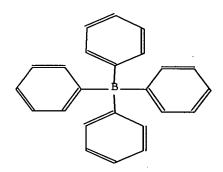
CM 1

FBRN 4160575 FMF C31 H35 P2



CM2

FBRN 3910925 FMF C24 H20 B



Fragment Notes:
Unknown location for Localized Charge of (-1)

Field Availability:

Code	Name	Occurrence
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FMF	Fragment Molecular Formula	2
MF	Molecular Formula	1
FW	Formular Weight	2
FBRN	Fragment BRN	2
LN	Lawson Number	4
FS	File Segment	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1

DED	Entry Date	1
DUPD	Update Date	1
CDISP	Compound Disposition	1
MP	Melting Point	1

All References:

ALLREF

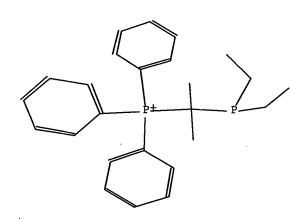
 Issleib, K.; Lindner, R., Justus Liebigs Ann. Chem., CODEN: JLACBF, 699, <1966>, 40-52

L51 ANSWER 21 OF 24 BEILSTEIN COPYRIGHT 2007 BEILSTEIN MDL on STN

Beilstein Records (BRN): 6710813 Lin. Struct. Formula (LSF): C25H31P2(1+)*C24H20B(1-)C25 H31 P2 , C24 H20 B Fragm. Molec. Formula (FMF): Molecular Formula (MF): C25 H31 P2 . C24 H20 B Molecular Weight (MW): 393.47, 319.23 Fragment BRN (FBRN): 6703356, 1654829 Lawson Number (LN): 16763, 16731, 3746, 709 Compound Type (CTYPE): isocyclic Constitution ID (CONSID): 5866315 Tautomer ID (TAUTID): 6431776 Beilstein Citation (BSO): 5-16 Entry Date (DED): 1994/07/15 Update Date (DUPD): 1994/07/19

CM 1

FBRN 6703356 FMF C25 H31 P2



CM 2

FBRN 1654829 FMF C24 H20 B

Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	
LSF	Linearized Structure Formula	1
FMF	Fragment Molecular Formula	2
MF	Molecular Formula	1
FW	Formular Weight	2
FBRN	Fragment BRN	2
LN	Lawson Number	4
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
DED	Entry Date	1
DUPD	Update Date	1
MP	Melting Point	1

This substance also occurs in Reaction Documents:

Code	Name Occ	currence
=======		======
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

All References:

ALLREF

1. Issleib, K.; Lindner, R., Justus Liebigs Ann. Chem., CODEN: JLACBF, 713, <1968>, 12-29

L51 ANSWER 22 OF 24 BEILSTEIN COPYRIGHT 2007 BEILSTEIN MDL on STN

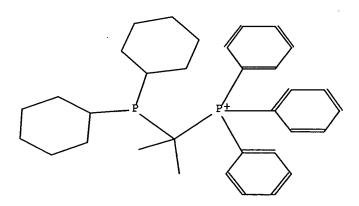
Beilstein Records (BRN): 4115452 Beilstein Pref. RN (BPR): 15389-64-7 CAS Reg. No. (RN): 15389-64-7 Chemical Name (CN): (2-Dicyclohexylphosphino-propyl) - (2) triphenylphosphonium-tetraphenyloborat Lin. Struct. Formula (LSF): C33H43P2(1+)*C24H20B(1-) Fragm. Molec. Formula (FMF): C33 H43 P2 , C24 H20 B Molecular Formula (MF): C33 H43 P2 . C24 H20 B Molecular Weight (MW): 501.65, 319.23

Fragment BRN (FBRN): 4163294, 1654829 Lawson Number (LN): 16763, 16731, 16723, 709 Compound Type (CTYPE): isocyclic Constitution ID (CONSID): 3768860 Tautomer ID (TAUTID): 4020027 Beilstein Citation (BSO): 5-16 Entry Date (DED): 1991/03/19 Update Date (DUPD):

1994/07/22

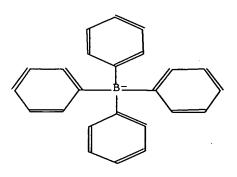
CM1

FBRN 4163294 FMF C33 H43 P2



CM 2

FBRN 1654829 FMF C24 H20 B



Field Availability:

Code Name Occurrence

BRN	Beilstein Records	1
BPR	Beilstein Preferred RN	1
RN	CAS Registry Number	1
CN	Chemical Name	1
LSF	Linearized Structure Formula	1
FMF	Fragment Molecular Formula	2
MF	Molecular Formula	1
FW	Formular Weight	2
FBRN	Fragment BRN	2
LN	Lawson Number	4
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
DED	Entry Date	1.
DUPD	Update Date	1
MP	Melting Point	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
=======		
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

All References:

ALLREF

 Issleib, K.; Lindner, R., Justus Liebigs Ann. Chem., CODEN: JLACBF, 713, <1968>, 12-29

L51 ANSWER 23 OF 24 BEILSTEIN COPYRIGHT 2007 BEILSTEIN MDL on STN

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Beilstein Records (BRN):
                                4109295
Chemical Name (CN):
                                Di-t.-butyl-o-isopropylphenylphosphin-
                                HBPh4
Lin. Struct. Formula (LSF):
                                C24H20B(1-)*C17H29P*H(1+)
Fragm. Molec. Formula (FMF):
                                C24 H20 B , C17 H29 P , H
Molecular Formula (MF):
                                C24 H20 B . C17 H29 P . H
Molecular Weight (MW):
                                319.23, 264.39, 1.01
Fragment BRN (FBRN):
                                1654829, 2939337, 3902898
Lawson Number (LN):
                                16763, 16728, 3758
Compound Type (CTYPE):
                                isocyclic
Constitution ID (CONSID):
                                3766274
Tautomer ID (TAUTID):
                                4013332
Beilstein Citation (BSO):
                                5-16
Entry Date (DED):
                                1991/03/19
Update Date (DUPD):
                                1991/09/02
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CM 1

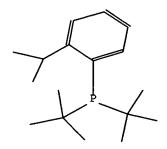
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FMF H

CM 2

FBRN 2939337

FMF C17 H29 P



CM 3

FBRN 1654829 FMF C24 H20 B

Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
LSF	Linearized Structure Formula	1
FMF	Fragment Molecular Formula	3
MF '	Molecular Formula	1
FW	Formular Weight	3
FBRN	Fragment BRN	3
LN	Lawson Number	3
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
DED	Entry Date	1
DUPD	Update Date	1
ELE	Electrical Data (MCS)	1
MP	Melting Point	1
NMR	Nuclear Magnetic Resonance	1

All References: ALLREF

1. Gill et al., J.Chem.Soc.Dalton Trans., CODEN: JCDTBI, <1973>, 270,272

1991/09/02

L51 ANSWER 24 OF 24 BEILSTEIN COPYRIGHT 2007 BEILSTEIN MDL on STN

Beilstein Records (BRN):
Chemical Name (CN):
Lin. Struct. Formula (LSF):
Fragm. Molec. Formula (FMF):
Molecular Formula (MF):
Molecular Weight (MW):
Fragment BRN (FBRN):
Lawson Number (LN):
Compound Type (CTYPE):
Constitution ID (CONSID):
Tautomer ID (TAUTID):
Beilstein Citation (BSO):
Entry Date (DED):
Update Date (DUPD):

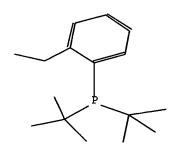
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Di-t.-butyl-o-ethylphenylphosphin-HBPh4
C24H20B(1-)*C16H27P*H(1+)
C24 H20 B , C16 H27 P , H
C24 H20 B . C16 H27 P . H
319.23, 250.36, 1.01
1654829, 2836338, 3902898
16763, 16734, 3758
isocyclic
3765873
4012726
5-16
1991/03/19

CM 1

FBRN 3902898 FMF H

CM 2

FBRN 2836338 FMF C16 H27 P



CM 3

FBRN 1654829 FMF C24 H20 B

Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	
RN	CAS Registry Number	2
CN	Chemical Name	1
LSF	Linearized Structure Formula	1
FMF	Fragment Molecular Formula	3
MF	Molecular Formula	1
FW	Formular Weight	3
FBRN	Fragment BRN	3
LN	Lawson Number	3
CTYPE	Compound Type	. 1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
DED	Entry Date	1
DUPD	Update Date	1
ELE	Electrical Data (MCS)	1
MP	Melting Point	1
NMR	Nuclear Magnetic Resonance	1

All References:

ALLREF

1. Gill et al., J.Chem.Soc.Dalton Trans., CODEN: JCDTBI, <1973>, 270,272

=> d his full

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(FILE 'HOME' ENTERED AT 11:46:47 ON 16 NOV 2007)
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FILE 'REGISTRY' ENTERED AT 11:47:07 ON 16 NOV 2007 STRUCTURE UPLOADED Ll L2 STRUCTURE UPLOADED L3 4 SEA SSS SAM L1 AND L2 D SCA 50 SEA SSS SAM L2 L425294 SEA SSS FUL L2 L_5 SAVE TEMP L5 NWA786STR2L/A L6 9567 SEA ABB=ON PLU=ON L5 AND P/ELS L7 4 SEA SUB=L5 SSS SAM L1 FILE 'STNGUIDE' ENTERED AT 11:52:18 ON 16 NOV 2007 FILE 'REGISTRY' ENTERED AT 11:56:18 ON 16 NOV 2007 rsSTRUCTURE UPLOADED T.9 4 SEA SUB=L5 SSS SAM L8 D SCA L10 47 SEA SUB=L5 SSS FUL L8 D SCA SAVE TEMP L10 NWA786STR8L/A SAVE TEMP L10 NWA699STR8L/A SAVE TEMP L5 NWA699STR2L/A DEL NWA786STR2L/A DEL NWA786STR8L/A ACT NWA699BPRNS/A

L11 (129) SEA ABB=ON PLU=ON (100-42-5/BI OR 100-47-0/BI OR 100-59-4/BI OR 10273-89-9/BI OR 105-56-6/BI OR 106-38-7/BI OR 106-99-0/BI OR 1066-54-2/BI OR 107-05-1/BI OR 107-15-3/BI OR 1078-71-3/BI OR 108-86-1/BI OR 108-90-7/BI OR 109-09-1/BI OR 109-69-3/BI OR 110-86-1/BI OR 111-85-3/BI OR 1122-91-4/BI OR 113279-72-4/BI OR 115-19-5/BI OR 122-39-4/BI OR 123-54-6/BI OR 131322-08-2/BI OR 13597-73-4/BI OR 13716-10-4/BI OR 13716-12-6/BI OR 143-66-8/ BI OR 15181-07-4/BI OR 15359-96-3/BI OR 155234-93-8/BI OR 15738-23-5/BI OR 1592-20-7/BI OR 16419-60-6/BI OR 16523-54-9/BI OR 200352-94-9/BI OR 2042-85-5/BI OR 20488-42-0/BI OR 20573-48-2/BI OR 224311-51-7/BI OR 2350-89-2/BI OR 25032-48-8/B I OR 2622-14-2/BI OR 2920-38-9/BI OR 29949-72-2/BI OR 2996-92-1 /BI OR 29965-97-7/BI OR 32673-25-9/BI OR 3375-31-3/BI OR 356518-17-7/BI OR 42092-01-3/BI OR 4553-07-5/BI OR 460-00-4/BI OR 501-65-5/BI OR 50704-04-6/BI OR 51364-51-3/BI OR 536-74-3/BI OR 538-58-9/BI OR 541-16-2/BI OR 542-18-7/BI OR 542-92-7/BI OR 56512-48-2/BI OR 56522-08-8/BI OR 5720-05-8/BI OR 586-77-6/B I OR 6002-40-0/BI OR 603-34-9/BI OR 603-35-0/BI OR 623-03-0/BI OR 629-04-9/BI OR 629-06-1/BI OR 629-20-9/BI OR 64-19-7/BI OR 643-58-3/BI OR 644-08-6/BI OR 6476-36-4/BI OR 6738-23-4/BI OR 6781-98-2/BI OR 72617-31-3/BI OR 74-85-1/BI OR 7439-89-6/BI OR 7439-95-4/BI OR 7439-96-5/BI OR 7440-02-0/BI OR 7440-05-3/BI OR 7440-06-4/BI OR 7440-16-6/BI OR 7440-18-8/BI OR 7440-48-4/BI OR 7459-73-6/BI OR 75-01-4/BI OR 75-05-8/BI OR 76-05-1/BI OR 7646-85-7/BI OR 7647-01-0/BI OR 7647-10-1/BI OR 7664-93-9/BI OR 77123-57-0/BI OR 7719-12-2/BI OR 78-86-4/BI OR 80-62-6/BI OR 81233-93-4/BI OR 853073-44-6/BI OR 853073-45-7/BI OR 853073-46-8/BI OR 853073-47-9/BI OR 853073-48-0/BI OR 853073-50

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-4/BI OR 853073-51-5/BI OR 853073-53-7/BI OR 853073-54-8/BI OR
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L12 (
             38) SEA ABB=ON PLU=ON L11 AND P/ELS
L13 (
             27) SEA ABB=ON PLU=ON L11 AND B/ELS
L14
             22 SEA ABB=ON PLU=ON L12 AND L13
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                ACT NWA699HITRNS/A
L15 (
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                OR 13597-73-4/BI OR 13716-10-4/BI OR 13716-12-6/BI OR 143-66-8/
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                /BI OR 29965-97-7/BI OR 32673-25-9/BI OR 3375-31-3/BI OR
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L16 (
             38) SEA ABB=ON PLU=ON L15 AND P/ELS
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L17 (
L18 (
             22) SEA ABB=ON PLU=ON L16 AND L17
L19 (
                                  .(20573-48-2/BI OR 131322-08-2/BI OR
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L20
             19 SEA ABB=ON PLU=ON L18 NOT L19
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L21
             21 SEA ABB=ON PLU=ON L10 AND L14
L22
              1 SEA ABB=ON PLU=ON L14 NOT L21
                D SCA
L23
              2 SEA ABB=ON PLU=ON L21 NOT L20
                D SCA
L24
             45 SEA ABB=ON PLU=ON L10 NOT L23
     FILE 'ZCAPLUS' ENTERED AT 12:05:19 ON 16 NOV 2007
L25
             18 SEA ABB=ON PLU=ON L24
               ACT NWA699AU1/A
L26
            104 SEA ABB=ON PLU=ON MASAOKA S?/AU
               ACT NWA699AU2/A
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10/580699
L27 6 SEA ABB=ON PLU=ON IWAZAKI H?/AU
L28 1 SEA ABB=ON PLU=ON L26 AND L27 L29 1 SEA ABB=ON PLU=ON L26 AND L25 D AU
L30
FILE 'BEILSTEIN' ENTERED AT 12:08:18 ON 16 NOV 2007 L34
FILE 'BABS' ENTERED AT 12:09:51 ON 16 NOV 2007 L39 4 SEA ABB=ON PLU=ON (6281441/BABSAN OR 6594776/BABSAN OR 6580383/BABSAN OR 6432734/BABSAN)
FILE 'ZCAPLUS, BABS' ENTERED AT 12:10:04 ON 16 NOV 2007 L40 19 DUP REM L25 L39 (3 DUPLICATES REMOVED) ANSWERS '1-18' FROM FILE ZCAPLUS ANSWER '19' FROM FILE BABS
FILE 'BEILSTEIN' ENTERED AT 12:10:20 ON 16 NOV 2007 L41 7 SEA ABB=ON PLU=ON L37 NOT L38 L42 1 SEA ABB=ON PLU=ON L41 AND RN/FA
FILE 'REGISTRY' ENTERED AT 12:13:07 ON 16 NOV 2007
FILE 'ZCAPLUS' ENTERED AT 12:13:11 ON 16 NOV 2007 D STAT QUE L28 D STAT QUE L32
FILE 'WPIX' ENTERED AT 12:13:31 ON 16 NOV 2007 L43 1 SEA ABB=ON PLU=ON L26 AND L27
FILE 'ZCAPLUS' ENTERED AT 12:13:51 ON 16 NOV 2007 L44 3 SEA ABB=ON PLU=ON L28 OR L32
FILE 'ZCAPLUS, WPIX' ENTERED AT 12:14:06 ON 16 NOV 2007 L45 3 DUP REM L44 L43 (1 DUPLICATE REMOVED) ANSWERS '1-3' FROM FILE ZCAPLUS D IBIB ABS HITIND HITSTR L45 1-3
FILE 'REGISTRY' ENTERED AT 12:14:58 ON 16 NOV 2007
FILE 'ZCAPLUS' ENTERED AT 12:15:02 ON 16 NOV 2007 D STAT QUE L28 D STAT QUE L32 L46 2 SEA ABB=ON PLU=ON (L26 OR L31) AND L25
FILE 'WPIX' ENTERED AT 12:15:52 ON 16 NOV 2007 D STAT QUE L43
FILE 'ZCAPLUS' ENTERED AT 12:16:12 ON 16 NOV 2007 L47

L48

FILE 'ZCAPLUS, WPIX' ENTERED AT 12:16:30 ON 16 NOV 2007

4 DUP REM L47 L43 (1 DUPLICATE REMOVED)

ANSWERS '1-4' FROM FILE ZCAPLUS
D IBIB ABS HITIND HITSTR L48 1-4

FILE 'REGISTRY' ENTERED AT 12:17:47 ON 16 NOV 2007

FILE 'ZCAPLUS' ENTERED AT 12:17:51 ON 16 NOV 2007

D STAT QUE L25

L49 4 SEA L48

L50 16 SEA ABB=ON PLU=ON L25 NOT L49

FILE 'BABS' ENTERED AT 12:18:50 ON 16 NOV 2007 D STAT QUE L39

FILE 'BEILSTEIN' ENTERED AT 12:19:02 ON 16 NOV 2007 D STAT QUE L41

FILE 'ZCAPLUS, BABS, BEILSTEIN' ENTERED AT 12:19:19 ON 16 NOV 2007 L51 24 DUP REM L50 L39 L41 (3 DUPLICATES REMOVED)

ANSWERS '1-16' FROM FILE ZCAPLUS ANSWER '17' FROM FILE BABS ANSWERS '18-24' FROM FILE BEILSTEIN

D IBIB ABS HITSTR L51 1-16

D IALL L51 17

D IDE ALLREF L51 18-24

FILE HOME

FILE REGISTRY

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 15 NOV 2007 HIGHEST RN 953991-83-8 DICTIONARY FILE UPDATES: 15 NOV 2007 HIGHEST RN 953991-83-8

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TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

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http://www.cas.org/support/stngen/stndoc/properties.html

FILE STNGUIDE

FILE CONTAINS CURRENT INFORMATION.

LAST RELOADED: Nov 9, 2007 (20071109/UP).

FILE ZCAPLUS

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FILE COVERS 1907 - 16 Nov 2007 VOL 147 ISS 22 FILE LAST UPDATED: 15 Nov 2007 (20071115/ED)

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This file contains CAS Registry Numbers for easy and accurate substance identification.

FILE BEILSTEIN
FILE LAST UPDATED ON September 26, 2007

FILE COVERS 1771 TO 2007.

FILE CONTAINS 10.119,480 SUBSTANCES

>>>PLEASE NOTE: Reaction Data and substance data are stored in separate documents and can not be searched together in one query. Reaction data for BEILSTEIN compounds may be displayed immediately with the display codes PRE (preparations) and REA (reactions). A substance answer set retrieved after the search for a chemical name, a compounds with available reaction information by combining with PRE/FA, REA/FA or more generally with RX/FA. The BEILSTEIN Registry Number (BRN) is the link between a BEILSTEIN compound and belonging reactions. For mo detailed reaction searches BRNs can be searched as reaction partner BRNs Reactant BRN (RX.RBRN) or Product BRN (RX.PBRN).<<<

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- * PLEASE NOTE THAT THERE ARE NO FORMATS FREE OF COST.
- * SET NOTICE FEATURE: THE COST ESTIMATES CALCULATED FOR SET NOTICE
- * ARE BASED ON THE HIGHEST PRICE CATEGORY. THEREFORE; THESE
- * ESTIMATES MAY NOT REFLECT THE ACTUAL COSTS.
- * FOR PRICE INFORMATION SEE HELP COST

- * PATENT NUMBERS (PN) AND BABS ACCESSION NUMBERS (BABSAN) CAN NOW BE SEARCHED, SELECTED AND TRANSFERRED.
- * NEW DISPLAY FORMATS ALLREF, ALLP AND BABSAN SHOW ALL REFERENCES, ALL PATENT REFERENCES, OR ALL BABS ACCESSION NUMBERS FOR A COMPOUND AT A GLANCE.

FILE BABS

FILE LAST UPDATED: 25 JUN 2007 <20070625/UP> FILE COVERS 1980 TO DATE.

FILE WPIX

FILE LAST UPDATED: 13 NOV 2007 <20071113/UP>
MOST RECENT THOMSON SCIENTIFIC UPDATE: 200773 <200773/DW>
DERWENT WORLD PATENTS INDEX SUBSCRIBER FILE, COVERS 1963 TO DATE

>>> IPC Reform backfile reclassification has been loaded to September 6th

=>

2007. No update date (UP) has been created for the reclassified documents, but they can be identified by 20060101/UPIC and 20061231/UPIC, 20070601/UPIC and 20071001/UPIC. <<<

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